Marches quantiques et mécanique quantique relativiste

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A Sofita.

Y a todas las personas que, llegadas a la edad adulta,
siguen cautivándose por ese edificio en eterna construcción
que llamamos Ciencia.

Foreword / *Agradecimientos*

This adventure started at some bar around Pocitos (Montevideo), Pablo had invited me to discuss about my interest in applying to France. Pointing to the rhombic tiling of the ceiling –it looked, after all, not too different to what two years later would become Fig. 3.3.4–, he would talk about rigorous results in quantum cellular automata and their connection to continuum physics, space-time, symmetries, and open problems. I thank Pablo for his continuous guidance.

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Abstract

This thesis is devoted to the development of two well-known models of computation for their application in quantum computer simulations. These models are the quantum walk (QW) and quantum cellular automata (QCA) models, and they constitute doubly strategic topics in this respect. First, they are privileged mathematical settings in which to encode the description of the actual physical system to be simulated. Second, they offer an experimentally viable architecture for actual physical devices performing the simulation.

For QWs, we prove precise error bounds and convergence rates of the discrete scheme towards the Dirac equation, thus validating the QW as a quantum simulation scheme. Furthermore, for both models we formulate a notion of discrete Lorentz covariance, which admits a diagrammatic representation in terms of local, circuit equivalence rules. We also study the continuum limit of a wide class of QWs, and show that it leads to a class of PDEs which includes the Hamiltonian form of the massive Dirac equation in (1+1)-dimensional curved spacetime.

Finally, we study the two particle sector of a QCA. We find the conditions for the existence of discrete spectrum (interpretable as molecular binding) for short-range and for long-range interactions. This is achieved using perturbation techniques of trace class operators and spectral analysis of unitary operators.

Résumé

Cette thèse étudie deux modèles de calcul: les marches quantiques (QW) et les automates cellulaires quantiques (QCA), en vue de les appliquer en simulation quantique. Ces modèles ont deux avantages stratégiques pour aborder ce problème: d'une part, ils constituent un cadre mathématique privilégié pour coder la description du système physique à simuler; d'autre part, ils correspondent à des architectures expérimentalement réalisables.

Nous effectuons d'abord une analyse des QWs en tant que schéma numérique pour l'équation de Dirac, en établissant leur borne d'erreur globale et leur taux de convergence. Puis nous proposons une notion de transformée de Lorentz discrète pour les deux modèles, QW et QCA, qui admet une représentation diagrammatique s'exprimant par des règles locales et d'équivalence de circuits. Par ailleurs, nous avons caractérisé la limite continue d'une grande classe de QWs, et démontré qu'elle correspond à une classe d'équations aux dérivées partielles incluant l'équation de Dirac massive en espace-temps courbe de $(1+1)$-dimensions.

Finalement, nous étudions le secteur à deux particules des automates cellulaires quantiques. Nous avons trouvé les conditions d'existence du spectre discret (interprétable comme une liaison moléculaire) pour des interactions à courte et longue portée, à travers des techniques perturbatives et d'analyse spectrale des opérateurs unitaires.

List of contributions

Refereed publications

1. The theoretical analysis of the Dirac QW presented in Chapter 2 was published in Journal of Physics A: Mathematical and Theoretical [ANF14] in collaboration with Pablo Arrighi and Vincent Nesme.

2. The Lorentz covariant interpretation of QWs and QCAs presented in Chapter 3 was published in New Journal of Physics [AFF14] in collaboration with Pablo Arrighi and Stefano Facchini.

3. The construction of Paired QWs for simulating non-homogeneous PDEs presented in Chapter 4 is available at [AFF15]. It has been submitted for publication, and it is co-authored with Pablo Arrighi and Stefano Facchini.

4. The spectral properties of interacting QWs presented in Chapter 5 is the object of a future publication [For15].

Communications

1. (a) "Journées Informatique Quantique" held at Nancy, France (2013), *The Dirac Quantum Walk* (talk);
   (b) Invited speaker at the Mathematics, Statistics and Applied Mathematics Seminar, NUI Galway, Ireland (2014), *The Cauchy problem for the continuous limit of Quantum Walks* (talk);
   (c) "Quantum walks and quantum simulations", Scuola Normale Superiore, Pisa, Italy (2013), *The Dirac equation as a Quantum Walk* (poster).

2. (a) "Colloque du GDR IQFA", quantum information conference held at Lyon, France (2014), *Discrete Lorentz covariance* (poster).

Conferences organized

We were in charge of the scientific and material organization of the meeting "Relativistic Quantum Walks" at Grenoble, France (6-7 février, 2014). There were 4 invited speakers and 7 contributed talks [GMRfr].

Contents

Chapter 1

Introduction

1.1 Context

QUANTUM computation can be defined as an interdisciplinary scientific field, devoted to understanding the computational power of physical systems in the quantum mechanical regime [NC10]. Among a great number of research directions, one is designing algorithms that cope with quantum mechanical laws, and hopefully outperform classical algorithms. In this respect, Quantum Walks (QWs) can be seen as the quantum mechanical analogue of classical random walks.

QWs were originally introduced [ADZ93, Mey96, AAKV01, Kem03] as dynamics having the following features:

- the underlying spacetime is a discrete grid;
- the evolution is unitary;
- it is causal, i.e. information propagates strictly at a bounded speed;
- it is homogeneous, i.e. translation-invariant and time-independent.

At the physical level, the design of actual hardware capable of performing QWs in the laboratory is an intense research area. We refer to the book [WM13] for an up-to-date discussion.

At the theoretical level, quantum computing has a number of algorithms that are phrased in terms of QWs, such as exponentially faster hitting [CCD$^+$03, FG98, CFG02], quantum search [Por13], and graph isomorphism [Kem03] to mention some; we refer to [VA12] for a review. The focus in this thesis is on QW models *per se*, or as models of a given quantum physical phenomena, through a continuum limit. In some sense this kind of approach is the one adopted by the very preliminary forms of QWs [SB93, BB94], around the 1990s. Nowadays, such QWs models are known to have a broad scope of applications:

- they provide discrete toy models to explore foundational questions [DP14, AFF14, AF13, FS14a, FS14b, Llo05];

- even for a classical computer they provide a stable numerical scheme, thereby guaranteeing convergence of the simulation as soon as the scheme is consistent [ANF14];
- they provide quantum algorithms, for the efficient simulation of the modelled phenomena upon a quantum simulation device [Fey82].

1.2 State of the art

Quantum simulation of the Dirac equation. The connection between QWs and the Dirac equation was first explored in [SB93, BB94, Mey96, BES07], and further developed in [D'A12, BDT13, Shi13, ANF14, FS14b, Str06b]. The non-relativistic Dirac to Shrödinger limit of the Dirac Quantum Walk is studied in [SB93, Str06a, Str06b, BT98a]. Decoherence, entanglement and Zitterbewegung are studied in [LB05, Str07]. The relationship with the Klein-Gordon equation is studied in [CBS10, dMD12]. The latter also studies the general continuous limit of one-dimensional space and time-dependent QWs. Similarly, [LB11, HJM^{+}05, FGLB12] provide variations aimed at accounting for the Maxwell-Dirac equations or the time-dependent Dirac equation, as well as faster convergence in numerical simulations. Algorithmic applications of the Dirac QW are studied in [CG04]. The issues of physical interpretation of the QW one-particle states are tackled in [BES07]. First principles derivations in $(1+1)$ and $(3+1)$-dimensions are provided in [BDT15, DP14]. The ideas behind the $(1+1)$-dimensional Dirac Quantum Walk can be traced back to Feynman's relativistic checkerboard [Bat12], although early models were not unitary [KN96] and sometimes continuous-time Ising-like [Ger81]. In $(2+1)$-dimensions, continuous-time models over the honeycomb lattice have been conceived in order to model electron transport in graphene [KTH08].

Lorentz covariance and discreteness. In physical theories, Lorentz *covariance* states that the laws of physics remain the same in all inertial frames. Lorentz *transforms* specify rules that serve to relate spacetimes as seen by different inertial frames. Clearly there is a problem with discreteness, since a fundamental discretization length (ε), can in principle be contracted as much as desired by a boost. Researchers have studied this apparent incompatibility from several angles. This is indeed an active area of research, both from the experimental [BG14] and from the epistemological sides [Hag14]. More recently, some communities have adopted an *informational* approach to this problem, and our contribution enters in this category. Let us present a brief summary of related works.

In the causal set approach, only the causal relations between the spacetime events is given. Without a background spacetime Lorentz covariance is vacuous. If, however, the events are generated from a Poissonian distribution over a flat spacetime, then covariance is recovered in a statistical sense [DHS04].

Researchers working on Lattice Boltzmann methods for relativistic hydrodynamics also take a statistical approach: the underlying model breaks Lorentz covariance, but the statistical distributions generated are covariant [MBHS10].

Loop Quantum Gravity offers a deep justification for the statistical approach. By interpreting spacetime intervals as the outcome of measurements of quantum mechanical operators, one can obtain covariance for the mean values, while keeping to a discrete spectrum [RS03, LO04].

The idea of interpreting space and time as operators with a Lorentz invariant discrete spectrum goes back to Snyder [Sny47]. This line of research goes under the name of Doubly Special Relativity (DSR). Relations between DSR and QWs are discussed in [BDBD$^+$15]. In the DSR approach, a deformation of the translational sector of the Poincaré algebra is required.

Instead of deforming the translation operator algebra, one could look at dropping translational invariance of the QW evolution. Along these lines, models have been constructed for QWs in external fields, including specific cases of gravitational fields [DMBD14, dMD12].

Another non-statistical, early approach is to restrict the class of allowed Lorentz transforms, to a subgroup of the Lorentz group whose matrices are over the integers numbers [Sch48]. Unluckily, there are no non-trivial integral Lorentz transforms in (1+1)-dimensions. Moreover, interaction rules that are covariant under this subgroup are difficult to find [HNO90, Das60].

Towards curved spacetime. The extension of to curved spacetime of QWs was initiated in [DMBD13, DMBD14, SFGP15]. In [DMBD13, DMBD14], Di Molfetta et al. have systematically studied the continuum limit of a two-time-step QW with arbitrary coin. This stroboscopic approach made it possible to recover the $(1+1)$-Weyl equation in curved spacetime, for metrics of having $g_{00} = 1$. This forbids the Schwarzschild metric for instance, but black holes can still be dealt with under suitable change of coordinates.

Another approach, recently pursued by Succi et al. [SFGP15], is within the framework of lattice discretization of the relativistic quantum wave equation (quantum lattice boltzmann [Suc01]). The key observation is that the mass term can be recovered by extending the neighbourhood of the dynamical map. However, the existence of a parametrization for the unitary evolution in terms of the metric, has remained an open question.

Two-particle sector of QCA, or interacting quantum walks. The extension of the discrete-time QW to multiple walkers was first studied by Omar et al. in 2004 [OPSB06]. They studied a two-particle QW on the line, and proved that coin entanglement induces spatial correlations between the spatial degrees of freedom. In their case the QW is *non-interacting*, in the sense that the coins are homogeneous. This subject was pursued further in [BW11, ŠBK$^+$11, LZG$^+$13], and physically implemented in [SGR$^+$12]. One should recall that the non-interacting case is not trivial in quantum mechanics. Indeed, a system with multiple particles –even non-interacting– presents new interesting features that depart from classical mechanics: there is entanglement and there are quantum statistical aspects, such as distinguishability.

Besides, researchers have studied non-homogeneous QWs with a “defect”, i.e. assuming that the coin operator is everywhere the same and distinct at a fixed position. Two different approaches are the method of CMV matrices [KN07] (since the QW matrix is naturally CMV-shaped), see [CGMV12], and the method of generating functions [KŁS13]. Non-homogeneous quantum walks have also been studied under periodic coins [LS09, SK10], and shown numerically that in some circumstances the spectrum has behaviour similar to the self-simliar Hofstadter butterfly [Hof76].

Finally, in [AAM$^+$12] they consider the non-homogeneity of the coin as an interaction. In particular, they study the spectrum of an IQW with a zero range interaction. In this case $V(0) = e^{\mathrm{i}g} I_4$, and I_4 otherwise. They prove the presence of eigenvalues in the gaps of the continuous spectrum, interpreted as molecular binding. This phenomenon manifests itself in the joint probability distributions as peaks wich are close to each other even after a long time, and the wave-function decays exponentially in the relative position of the two particles.

1.3 Thesis outline

This thesis is organized as follows:

- In **Chapter 2**, we formally analyse the Dirac QW and obtain a result on the convergence of solutions of the discrete scheme towards the Dirac equation.
- In **Chapter 3**, we present a new framework for describing Lorentz covariance symmetry property of QWs and QCAs.
- In **Chapter 4** we introduce *Paired QWs*, which are both a subclass of the general QWs described above, and generalization of the most usual QWs found in the literature.
- In **Chapter 5**, we study interacting QWs (IQWs), i.e. the two-particle sector of a QCA. We perform a thorough analysis of the spectral properties of the free walk, and then treat the interacting case as a perturbation problem.
- In **Chapter 6** we draw the main conclusions and we suggest some interesting future lines of research.

Chapter 2

The Dirac quantum walk

FOR the purpose of quantum simulation (on a quantum device) as envisioned by Feynman [Fey82], or for the purpose of exploring the power and limits of discrete models of physics, we may wish to discretize the Dirac equation. There are (at least) two directions one could follow. First, through finite-difference methods; the problem with this approach is that the discrete scheme does not conserve the $||.||_2$-norm, in general, hence violating unitarity. The second approach would be integrating exactly the Dirac equation; the transformation would be unitary, but it is unclear how to discretize space. In this chapter, we solve both problems by proving convergence of solutions of a class of QWs towards the solution of the Cauchy problem of the Dirac equation. We do so by adapting a powerful method from standard numerical analysis, which is of general interest to the field of quantum simulation.

We start introducing the Dirac equation and review related works in Section 2.1. In Section 2.2 we find the class of QWs with the desired properties, that are investigated in the subsequent sections. We continue with the formal analysis of the discrete scheme in Section 2.3, setting the notation and including some mathematical preliminaries from Fourier analysis and Sobolev spaces. We then recall the well-posedness of the Dirac equation in Section 2.4, and prove that our discrete scheme is consistent (Section 2.5), stable (Section 2.6), and finally, convergent (Section 2.7). We conclude with a result on the global error including space discretization (Section 2.8), and summarize in Section 2.9.

2.1 Introduction

2.1.1 Discretization approaches of the Dirac equation

The Dirac equation is a partial differential equation, first order in time, and it is of central importance for describing relativistic quantum particles [BD64, Tha92]. For a free fermion of mass m, it takes the form[1]:

$$\mathrm{i}\partial_0\psi = D\psi, \quad \text{with} \quad D = m\alpha^0 - \mathrm{i}\sum_j \alpha^j\partial_j, \tag{2.1.1}$$

[1]We always work in Planck units, $\hbar = c = 1$.

where the Latin index j spans the spatial dimensions $1 \dots n$, with $1 \leq n \leq 3$, and whereas Greek indices μ, ν will span the space-time dimensions $0 \dots n$. The domain of definition of the operator D is made precise in Section 2.4; for the moment, we think of ψ in (2.1.1) as a differentiable space-time wave-function from $\mathbb{R}^{n+1}$ to $\mathbb{C}^d$, with d a number that depends on n, whereas ϕ will denote a space-like wave-function from $\mathbb{R}^n$ to $\mathbb{C}^d$, e.g. we may write $\phi = \psi(x_0 = 0)$ for the initial state. Finally, the (α^μ) are $d \times d$ hermitian matrices which must verify $\alpha^\mu \alpha^\nu - \alpha^\nu \alpha^\mu = 2\delta_{\mu\nu} \operatorname{Id}$, i.e. they square to the identity and pairwise anticommute [Tha92]. Physically, the integer d encodes the *spinor* nature of a Dirac-like particle, and it is either 2 or 4 for the applications we will consider.

There are (at least) two obvious directions one could follow to discretize the Dirac equation. First, through finite-difference methods one gets (where $\tau_{\mu,\varepsilon}$ denotes translation by ε along the μ-axis):

$$\psi(x_0 + \varepsilon) = (\operatorname{Id} - \mathrm{i}\varepsilon D_\varepsilon)\psi(x_0), \tag{2.1.2}$$

$$\text{with} \quad D_\varepsilon = m\alpha^0 - \mathrm{i}\sum_j \alpha^j \frac{\tau_{j,\varepsilon} - \operatorname{Id}}{\varepsilon}, \tag{2.1.3}$$

$$(\tau_{\mu,\varepsilon}\psi)(x_\mu) = \psi(x_\mu + \varepsilon). \tag{2.1.4}$$

The problem with this crude approach is that $(\operatorname{Id} - \mathrm{i}\varepsilon D_\varepsilon)$ does not conserve the $||.||_2$-norm, in general. From the point of view of numerical simulation, this means one has to check the model's convergence and stability. From the point of view of quantum simulation this simply bars the model as not implementable on a quantum simulating device. From the point of view of discrete toy models of physics, this means that the model lacks one of the fundamental, guiding symmetries: unitarity.

The second approach would be integrating exactly the original Dirac equation, and expressing $\psi(x_0 + \varepsilon)$ as a function of $\psi(x_0)$. The transformation would be unitary, but it is unclear how to discretize space.

2.1.2 Motivations and related works

In numerical analysis, in order to evaluate the quality of a numerical scheme, two main criteria are used. The first criterion is consistency, a.k.a. accuracy. Intuitively it demands that, after an ε of time, the discrete model approximates the solution to a given order of ε.

Consistency of the $(1+1)$-dimensional Dirac QW has been argued in [Mey96], and for the $(1+1)$-dimensional massless case in [CBS10]. It has been observed numerically in $(1+1)$-dimensions in [LB05] and in $(3+1)$-dimensions in [Pal09, LD11, DLPS11]. It has been proved in $(1+1)$-dimensions in [Str06b, Str07, BDT15].

The second criterion is convergence. Intuitively it demands that, after an arbitrary time x_0, and if ε was chosen small enough, the discrete model approximates the solution to a given order of ε. This criterion is stronger[2]. Convergence has been observed numerically

[2] Of course convergence implies consistency, but the converse does not always hold. Indeed, consistency means that making ε small will increase the precision of the simulation of an ε of time step. But it will also increase the number of time steps $l = x_0/\varepsilon$ which are required in order to simulate an x_0 of time evolution. Depending upon whether the two effects compensate, convergence may or may not be reached.

in $(3+1)$-dimensions in [Pal09, LD11, DLPS11]. It has been proved in $(1+1)$-dimensions in [Str06b, Str07, Shi13]. The difficulty to analyse the $(3+1)$-dimensional Dirac QW is mentioned in [Str06a, Str07, BT98b, Cha11].

2.2 Construction of the Dirac QW

2.2.1 In $(2+1)$-dimensions

A standard representation of the $(2+1)$-dimensional Dirac equation is:

$$\mathrm{i}\partial_0\psi = D\psi \quad \text{with} \quad D = m\sigma^2 - \mathrm{i}\sigma^1\partial_1 - \mathrm{i}\sigma^3\partial_2 \tag{2.2.1}$$

and (σ^μ) the Pauli matrices, with σ^0 the identity, i.e.

$$\sigma^0 = \begin{pmatrix}1 & 0\\ 0 & 1\end{pmatrix}, \ \sigma^1 = \begin{pmatrix}0 & 1\\ 1 & 0\end{pmatrix}, \ \sigma^2 = \begin{pmatrix}0 & -\mathrm{i}\\ \mathrm{i} & 0\end{pmatrix}, \ \sigma^3 = \begin{pmatrix}1 & 0\\ 0 & -1\end{pmatrix}. \tag{2.2.2}$$

Now, intuitively,

$$\tau_{\mu,\varepsilon}\psi = (\mathrm{Id} + \varepsilon\partial_\mu)\psi + O(\varepsilon^2). \tag{2.2.3}$$

but this statement and its hypotheses will only be made formal and quantified in later sections. Meanwhile, substituting Eq. (2.2.1) into Eq. (2.2.3) for $\mu = 0$ yields:

$$\begin{aligned}\tau_{0,\varepsilon} &= (\mathrm{Id} - \mathrm{i}\varepsilon D) + O(\varepsilon^2)\\ &= (\mathrm{Id} - \mathrm{i}\varepsilon m\sigma^2)(\mathrm{Id} - \varepsilon\sigma^1\partial_1)(\mathrm{Id} - \varepsilon\sigma^3\partial_2) + O(\varepsilon^2)\\ &= \exp\left(-\mathrm{i}\varepsilon m\sigma^2\right) H(\mathrm{Id} - \varepsilon\sigma^3\partial_1)H(\mathrm{Id} - \varepsilon\sigma^3\partial_2) + O(\varepsilon^2)\end{aligned} \tag{2.2.4}$$

since $\sigma^1 = H\sigma^3 H$ with H the Hadamard gate, $H = \frac{1}{\sqrt{2}}\begin{pmatrix}1 & 1\\ 1 & -1\end{pmatrix}$. Using the definition of σ^3, using Eq. (2.2.3), and taking the convention that $\mathbb{C}^2$ is spanned by the orthonormal basis $\{|l\rangle / l \in \{-1,1\}\}$, we get:

$$\tau_{0,\varepsilon} = C_\varepsilon H T_{1,\varepsilon} H T_{2,\varepsilon} + O(\varepsilon^2) \tag{2.2.5a}$$

$$\text{with} \quad C_\varepsilon = \exp\left(-\mathrm{i}\varepsilon m\sigma^2\right) \tag{2.2.5b}$$

$$\text{and} \quad T_{j,\varepsilon} = \sum_{l\in\{-1,1\}} |l\rangle\langle l|\tau_{j,l\varepsilon}. \tag{2.2.5c}$$

Overall, we have:

$$\psi(x_0 + \varepsilon) = W_\varepsilon\psi(x_0) + O(\varepsilon^2) \tag{2.2.6a}$$

$$\text{with} \quad W_\varepsilon = C^\varepsilon H T_{1,\varepsilon} H T_{2,\varepsilon} \tag{2.2.6b}$$

where the T matrices are partial shifts. This Dirac Quantum Walk [SB93, BB94, Mey96] models the $(2+1)$-dimensional Dirac equation. It has a product form. Such 'alternate quantum walks' have the advantage of using a two-dimensional coin-space instead of a four-dimensional coin-space: fewer resources are needed for their implementation [DFMGMB11]. It is still just one quantum walk, i.e. a translation-invariant causal unitary operator.

2.2.2 In $(3+1)$-dimensions

From $(2+1)$ to $(3+1)$-dimensions the Dirac equation changes form, the spin degree of freedom goes to degree four. The equation is:

$$\begin{aligned} \mathrm{i}\partial_0\psi &= D\psi \quad \text{with} \\ D &= m(\sigma^2 \otimes \sigma^0) + \mathrm{i}\sum_j (\sigma^3 \otimes \sigma^j)\partial_j \end{aligned} \tag{2.2.7}$$

Indeed, one can check that the matrices $\sigma^2 \otimes \sigma^0$ and $-\sigma^3 \otimes \sigma^i$ are hermitian, that they square to the identity, and that they anticommute. Using the definition of σ^3, Eq. (2.2.3), and taking the convention that $\mathbb{C}^4$ is spanned by the orthonormal basis $\{|r,l\rangle \,/\, r,l \in \{-1,1\}\}$:

$$\left(\mathrm{Id} + \varepsilon(\sigma^3 \otimes \sigma^3)\partial_3\right)\psi = T_{3,\varepsilon}\psi + O(\varepsilon^2) \tag{2.2.8a}$$

$$\text{with} \quad T_{j,\varepsilon} = \sum_{r,l\in\{-1,1\}} |r,l\rangle\langle r,l|\tau_{j,rl\varepsilon}. \tag{2.2.8b}$$

Similarly,

$$\left(\mathrm{Id} + \varepsilon(\sigma^3 \otimes \sigma^2)\partial_2\right)\psi = (\mathrm{Id} \otimes F)T_{2,\varepsilon}(\mathrm{Id} \otimes F^\dagger)\psi + O(\varepsilon^2) \tag{2.2.9a}$$

$$\text{as} \quad \sigma^2 = F\sigma^3 F^\dagger \tag{2.2.9b}$$

$$\text{with} \quad F = R_{\frac{\pi}{2}} H = \begin{pmatrix} 1/\sqrt{2} & 1/\sqrt{2} \\ \mathrm{i}/\sqrt{2} & -\mathrm{i}/\sqrt{2} \end{pmatrix}. \tag{2.2.9c}$$

Likewise,

$$\left(\mathrm{Id} + \varepsilon(\sigma^3 \otimes \sigma^1)\partial_1\right)\psi = (\mathrm{Id} \otimes H)T_{1,\varepsilon}(\mathrm{Id} \otimes H)\psi + O(\varepsilon^2) \tag{2.2.10a}$$

$$\text{as} \quad \sigma^1 = H\sigma^3 H. \tag{2.2.10b}$$

Finally, let $C_\varepsilon = \exp\left(-\mathrm{i}\varepsilon m(\sigma^2 \otimes \sigma^0)\right)$. We have:

$$\psi(x_0 + \varepsilon) = W_\varepsilon \psi(x_0) + O(\varepsilon^2), \tag{2.2.11}$$

with

$$W_\varepsilon = C_\varepsilon(\mathrm{Id} \otimes H)T_{1,\varepsilon}(\mathrm{Id} \otimes HF)T_{2,\varepsilon}(\mathrm{Id} \otimes F^\dagger)T_{3,\varepsilon} \tag{2.2.12}$$

where the T matrices are partial shifts. This is the $(3+1)$-dimensional Dirac Quantum Walk. We now move on to the formal analysis of the model.

2.3 Mathematical preliminaries

We begin the formal analysis of the discrete scheme with a review of some standard mathematical facts, namely from Fourier analysis and Sobolev spaces. They also serve to fix notation for the following sections.

2.3.1 Fourier transform

We recall that the Fourier transform of the wave-function $\phi \in L^2(\mathbb{R}^n)^d$ is defined as the function $(\mathcal{FT}\phi) = \hat{\phi} : \mathbb{R}^n \to \mathbb{C}^d$ such that

$$\hat{\phi}(k) = \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} \phi(x) e^{-ik\cdot x}\,\mathrm{d}x \tag{2.3.1}$$

where by $k \cdot x$ we mean the scalar product in Euclidean space $\mathbb{R}^n$, $x = (x_j)$, and $k = (k_j)$. The function $\mathcal{FT}$ is unitary, its inverse is

$$\phi(x) = \frac{1}{(2\pi)^{n/2}} \int_{\mathbb{R}^n} \hat{\phi}(k) e^{ik\cdot x}\,\mathrm{d}k. \tag{2.3.2}$$

From the above definition it is easily seen that for the spatial derivatives: $\mathcal{FT}(\partial_j \phi)(k) = ik_j\hat{\phi}$. Is is also useful to recall that for translations:

$$\mathcal{FT}\left(\phi(x \pm \varepsilon)\right)(k) = e^{\pm \mathrm{i}k\cdot\varepsilon}\,\hat{\phi}(k). \tag{2.3.3}$$

In Fourier space the $(2+1)$-dimensional Dirac operator, Eq. (2.2.1), becomes:

$$\begin{aligned}\hat{D}(k) &= m\sigma^2 + k_1\sigma^1 + k_2\sigma^3 \\ &= \begin{pmatrix} k_2 & k_1 - \mathrm{i}m \\ k_1 + \mathrm{i}m & -k_2 \end{pmatrix}\end{aligned} \tag{2.3.4}$$

with eigenvalues $\pm|\gamma|$, being $\gamma^2 = m^2 + ||k||^2$. The same formula for the eigenvalues holds true in three dimensions (i.e. there is a twofold degeneracy).

In Fourier space the $(2+1)$-dimensional Dirac Quantum Walk operator $\hat{W}_\varepsilon$, decomposes as a product of exponential matrices, using identities such as:

$$H\hat{T}_{1,\varepsilon}(k)H = H\begin{pmatrix} e^{-\mathrm{i}k_1\varepsilon} & 0 \\ 0 & e^{\mathrm{i}k_1\varepsilon} \end{pmatrix}H = He^{-\mathrm{i}k_1\varepsilon\sigma^3}H = e^{-\mathrm{i}\varepsilon k_1\sigma^1} \tag{2.3.5}$$

and likewise for the other directions. Eventually in $(n+1)$-dimensions it takes the form

$$\hat{W}_\varepsilon = \prod_\mu e^{-\mathrm{i}\varepsilon\hat{A}_\mu} \tag{2.3.6}$$

with some known $\hat{A}_\mu$.

2.3.2 Fourier series

We recall that the Fourier series of the wave-function $\phi \in L^2([-\frac{\pi}{\varepsilon}, \frac{\pi}{\varepsilon}]^n)^d$, $\varepsilon \in \mathbb{R}^+$, is defined as the function $(\mathcal{FS}\phi) = \hat{\phi} : \varepsilon\mathbb{Z}^n \to \mathbb{C}^d$ such that

$$\hat{\phi}(k) = \left(\frac{\varepsilon}{2\pi}\right)^{n/2} \int_{[-\frac{\pi}{\varepsilon}, \frac{\pi}{\varepsilon}]^n} \phi(x) e^{ik\cdot x}\, \mathrm{d}x. \tag{2.3.7}$$

The function $\mathcal{FS}$ is unitary, its inverse is

$$\phi(x) = \left(\frac{\varepsilon}{2\pi}\right)^{n/2} \sum_{k\in\varepsilon\mathbb{Z}^n} \hat{\phi}(k) e^{-ik\cdot x}. \tag{2.3.8}$$

The sign conventions of the exponentials are slightly non-standard. They have been on purpose so that, whenever $\hat{\phi} = \mathcal{FT}(\phi)$ has support in $[-\frac{\pi}{\varepsilon}, \frac{\pi}{\varepsilon}]^n$, then (with $|_X$ denoting restriction to X):

$$\mathcal{FS}(\hat{\phi}|_{[-\frac{\pi}{\varepsilon}, \frac{\pi}{\varepsilon}]^n}) = \varepsilon^{n/2}\mathcal{FT}^{-1}(\hat{\phi})|_{\varepsilon\mathbb{Z}^n} = \varepsilon^{n/2}\phi|_{\varepsilon\mathbb{Z}^n}, \tag{2.3.9}$$

and

$$\mathcal{FS}^{-1}(\varepsilon^{n/2}\phi|_{\varepsilon\mathbb{Z}^n}) = \hat{\phi}|_{[-\frac{\pi}{\varepsilon}, \frac{\pi}{\varepsilon}]^n}. \tag{2.3.10}$$

Indeed, the (2.3.9) follows from the definition, and (2.3.10) is the reciprocal.

2.3.3 Sobolev spaces

The usual wave-function space for quantum theory is the subspace $L^2(\mathbb{R}^n)^d$ of the functions $\mathbb{R}^n \to \mathbb{C}^d$ for which the $||.||_2$-norm is finite. Recall that

$$||\phi||_2 = \sqrt{\int_{\mathbb{R}^n} ||\phi(x)||^2 \mathrm{d}x} \tag{2.3.11}$$

with $||.||$ the usual 2-norm in $\mathbb{C}^d$, and $x = (x_i)$. For our approximations to hold, we need to restrict to the (weighted) Sobolev space $H^s_m(\mathbb{R}^n)^d$ of the functions $L^2(\mathbb{R}^n)^d$ for which the $||.||_{H^s_m}$-norm is finite, for some fixed $s \geq 0$, $m \geq 0$. Here,

$$||\phi||_{H^s_m} = \sqrt{\int_{\mathbb{R}^n} (1 + m^2 + ||k||^2)^s ||\hat{\phi}(k)||^2 \mathrm{d}k} \tag{2.3.12}$$

with $\hat{\phi}$ the Fourier transform of ϕ, and $||k||^2 = \sum_j |k_j|^2$.

Several remarks are in order. First, notice that $||\phi||_{H^0_m} = ||\hat{\phi}||_2 = ||\phi||_2$, thus $H^0_m(\mathbb{R}^n)^d = L^2(\mathbb{R}^n)^d$. Second, notice that for continuous differentiable functions,

$$||\phi||^2_{H^1_m} = (1 + m^2)||\phi||^2_2 + \sum_j ||\partial_j\phi||^2_2, \tag{2.3.13}$$

thus $H^1_m(\mathbb{R}^n)^d$ is just the subset of $L^2(\mathbb{R}^n)^d$ having first-order derivatives in $L^2(\mathbb{R}^n)^d$, and it is often referred to as the energy norm. Second, $H^{s+1}_m(\mathbb{R}^n)^d$ is dense in $H^s_m(\mathbb{R}^n)^d$, as can be seen from mollification techniques [Sob38]. Finally, notice that, on the one hand, the choice of having the $||.||_{H^s_m}$-norm to depend on m is slightly non-standard: usually this constant is set to zero. On the other hand, three elements argue in favour of this non-standard choice:

1. It fits nicely with the mathematics of this approach;
2. Our main use of the $||.||_{H^{s>0}_m}$-norm is to impose a sufficiently regular initial condition on the particle's wave-function, that this regularity condition may depend on the particle's mass m does not seem problematic;
3. The above defined $||.||_{H^s_m}$-norm is equivalent to the usual $||.||_{H^s}$-norm:

$$||\phi||_{H^s} = \sqrt{\int_{\mathbb{R}^n} (1+||k||^2)^s ||\hat{\phi}(k)||^2 dk} \tag{2.3.14}$$

   in the sense of norm equivalence, because

$$1 + ||k||^2 \leq 1 + m^2 + ||k||^2 \leq (m^2+1)(1+||k||^2). \tag{2.3.15}$$

This last point is why the well-posedness of the Dirac equation with respect to the usual $||.||_{H^s}$-norm carries through with respect to the $||.||_{H^s_m}$-norm, see next section.

2.4 Well-posedness

A major concern in numerical analysis is finding discrete models to approximate the continuous solutions of a well-posed Cauchy problem. Here, the Cauchy problem is to find the solution ψ given $\psi(0)$ and $\mathrm{i}\partial_0\psi = D\psi$. Intuitively, Cauchy problems are well-posed if and only if the solution exists, is unique, and if small variations on the initial state $\psi(0)$ have a small impact on the final state $\psi(x_0)$. In mathematical terms, a Cauchy problem is *well-posed* in a Banach space X if:

- D is a densely defined operator on X, that is, Dom $D \subset X$ is a dense subset of X;
- There exists a dense subset Y of X such that for every initial condition in Y, the Cauchy problem has a solution;
- There exists a non-decreasing function $C : \mathbb{R}^+ \to \mathbb{R}^+$ such that for every $x_0 \in \mathbb{R}^+$, $||\psi(x_0)||_X \leq C(x_0)||\psi(0)||_X$ for any solution ψ (not necessarily from an initial condition in Y).

A symmetric hyperbolic system is a Cauchy problem of the form

$$\partial_0\psi = D\psi \quad \text{with} \quad D = -\mathrm{i}\beta^0 - \sum_j \beta^j \partial_j \tag{2.4.1}$$

where the (β^μ) are hermitian.

For symmetric hyperbolic systems, the Cauchy problem is known to be well-posed in $H^s(\mathbb{R}^n)^d$ for any $s \geq 0$. D is defined on the subspace of $H^s(\mathbb{R}^n)^d$ such that $D\phi \in H^s(\mathbb{R}^n)^d$ for any $\phi \in H^s(\mathbb{R}^n)^d$, which is dense indeed, and every initial condition in this space yields a solution. The H^s-norm is constant for solutions of the problem, so that $C(t) = 1$ fulfills the requirement. For references, see [Fat83] (1.6.21) or [BGS07].

Since the Dirac equation is a symmetric hyperbolic system, the problem is well-posed [Fat83] for the Sobolev space $H^s_m(\mathbb{R}^n)^d$, with $s \geq 0$ of the functions for which the $||.||_{H^s_m}$-norm is finite, with Sobolev norm given by (2.3.12). Notice that the Sobolev norm involves an integral in Fourier space. For this reason, and because the Dirac operator is just a pointwise multiplication in Fourier space, most of the following derivations will use the notation introduced in Section 2.3.

2.5 Consistency

In numerical analysis, in order to evaluate the quality of a numerical scheme, the first criterion is *consistency*, also known as accuracy. Intuitively it demands that, after an ε of time, the discrete model approximates the solution to a given order of ε.

Formally, say a Cauchy problem is well-posed on X, with Y a dense subspace of X. The discrete model W_ε is consistent of order r on Y if and only if there exists C such that for any solution ψ with $\psi(x_0 = 0) \in Y$, for all $\varepsilon \in \mathbb{R}^+$, we have

$$||W_\varepsilon \psi(0) - \psi(\varepsilon)||_X = \varepsilon^{r+1} C ||\psi(0)||_Y. \tag{2.5.1}$$

The main result of this section is the following.

Proposition 2.1. *For $s \geq 0$, $r = 1$, $X = H^s_m(\mathbb{R}^n)^d$ and $Y = H^{s+2}_m(\mathbb{R}^n)^d$, for all $\phi \in Y$, and for all $\varepsilon > 0$,*

$$||W_\varepsilon \phi - T(\varepsilon)\phi||_{H^s_m} \leq \varepsilon^2 C_n ||\phi||_{H^{s+2}_m}, \tag{2.5.2}$$

with $\phi = \psi(0)$, $T(\varepsilon)\phi = \psi(\varepsilon)$, i.e. $T(\varepsilon) = \tau_{0,\epsilon}$ is the continuous solution's time evolution operator, and $C_n = 1 + n/2$.

2.5.1 Proof of consistency

We work on Fourier space and see $\hat{W}_\varepsilon(k)$ with fixed k as a function of the real-valued ε. First, observe that the quantum walk operator can generally be written as (we sometimes omit the k dependence in the notations of this section):

$$\hat{W}_\varepsilon = \prod_\mu e^{-\mathrm{i}\varepsilon \hat{A}_\mu}, \tag{2.5.3}$$

see Subsection 2.3.1 where one such construction is made explicit. Here $\hat{A}_\mu$ are hermitian, $|||\hat{A}_0|||_2 = m$, $|||\hat{A}_j|||_2 = k_j$, and $\sum_\mu \hat{A}_\mu = \hat{D}$. For instance, in $(2+1)$-dimensions, $\hat{A}_0$ is equal to $m\sigma^2$, $\hat{A}_1$ is equal to $k_1\sigma^1$ and $\hat{A}_2$ is equal to $k_2\sigma^3$.

As $\hat{W}_\varepsilon(k)$ is a matrix whose elements are products of trigonometric functions and exponentials, its entries are $\mathcal{C}^\infty$ functions (on the variable ε). We will denote ∂_ε the derivative with respect to variable ε in each entry. Observe that $\hat{W}_0 = \mathrm{Id}$.

Now we calculate the first and second order derivatives making use of Eq. (2.5.3). For the first order derivative we have

$$\begin{aligned}\left(\partial_\varepsilon \hat{W}_\varepsilon\right)_\varepsilon &= \left(-\mathrm{i}\hat{A}_0\right) e^{-\mathrm{i}\varepsilon \hat{A}_0} \cdots e^{-\mathrm{i}\varepsilon \hat{A}_n} + e^{-\mathrm{i}\varepsilon \hat{A}_0} \left(-\mathrm{i}\hat{A}_1\right) e^{-\mathrm{i}\varepsilon \hat{A}_1} \cdots e^{-\mathrm{i}\varepsilon \hat{A}_n} + \cdots \\ &\qquad + e^{-\mathrm{i}\varepsilon \hat{A}_0} \cdots \left(-\mathrm{i}\hat{A}_n\right) e^{-\mathrm{i}\varepsilon \hat{A}_n} \\ &= \sum_\mu \left(\prod_{\kappa<\mu} e^{-\mathrm{i}\varepsilon \hat{A}_\kappa}\right) \left(-\mathrm{i}\hat{A}_\mu\right) \left(\prod_{\kappa\geq\mu} e^{-\mathrm{i}\varepsilon \hat{A}_\kappa}\right).\end{aligned} \tag{2.5.4}$$

Evaluating at $\varepsilon = 0$,

$$\left(\partial_\varepsilon \hat{W}_\varepsilon\right)_{\varepsilon=0} = -\mathrm{i}\hat{D}. \tag{2.5.5}$$

For the second order derivative, the computation is slightly more involved, but we can proceed similarly as in (2.5.4). The result after regrouping is

$$\begin{aligned}\left(\partial^2_\varepsilon \hat{W}_\varepsilon\right)_\varepsilon &= -\sum_\mu \left(\prod_{\kappa<\mu} e^{-\mathrm{i}\varepsilon \hat{A}_\kappa}\right) \hat{A}^2_\mu \left(\prod_{\kappa\geq\mu} e^{-\mathrm{i}\varepsilon \hat{A}_\kappa}\right) \\ &\quad - 2\sum_{\nu<\mu} \left(\prod_{\kappa<\nu} e^{-\mathrm{i}\varepsilon \hat{A}_\kappa}\right) \hat{A}_\nu \left(\prod_{\nu\leq\kappa<\mu} e^{-\mathrm{i}\varepsilon \hat{A}_\kappa}\right) \hat{A}_\mu \left(\prod_{\kappa\geq\mu} e^{-\mathrm{i}\varepsilon \hat{A}_\kappa}\right).\end{aligned} \tag{2.5.6}$$

Then,

$$\begin{aligned}|||\partial^2_\varepsilon \hat{W}_\varepsilon|||_2 &\leq \sum_\mu |||\hat{A}^2_\mu|||_2 + 2\sum_{\nu<\mu} |||\hat{A}_\nu|||_2 \, |||\hat{A}_\mu|||_2 \\ &\leq \left(\sum_\mu |||\hat{A}_\mu|||_2\right)^2 \\ &\leq (n+1)\sum_\mu |||\hat{A}_\mu|||_2^2\end{aligned} \tag{2.5.7}$$

where we get to the last line using that[3] for real numbers, $(x_0 + \cdots + x_n)^2 \leq (n+1)(x_0^2 + \cdots + x_n^2)$. Now, since $\gamma^2 = m^2 + ||k||_2^2$, then

$$|||\partial^2_\varepsilon \hat{W}_\varepsilon|||_2 \leq (n+1)\gamma^2. \tag{2.5.8}$$

By application of Taylor's formula with the integral form for the remainder [KL03] to each

[3]It is an easy consequence of the Cauchy-Bunyakovsky-Schwarz inequality for sums, that is, $\left(\sum_{k=1}^n a_k b_k\right)^2 \leq \left(\sum_{k=1}^n a_k^2\right)\left(\sum_{k=1}^n b_k^2\right)$ for arbitrary real numbers $(a_k)_{k=1}^n$ and $(b_k)_{k=1}^n$.

entry of the matrix $\hat{W}_\varepsilon$, we get

$$\hat{W}_\varepsilon = \mathrm{Id} + \varepsilon \left(\partial_\varepsilon \hat{W}_\varepsilon\right)_{\varepsilon=0} + \int_0^\varepsilon (\varepsilon - \eta) \left(\partial_\varepsilon^2 \hat{W}_\varepsilon\right)_{\varepsilon=\eta} d\eta \tag{2.5.9}$$

and

$$\hat{T}(\varepsilon) = e^{-\mathrm{i}\varepsilon\hat{D}} = \mathrm{Id} - \mathrm{i}\varepsilon\hat{D} + \int_0^\varepsilon (\varepsilon - \eta) \left(-\hat{D}^2 e^{-\mathrm{i}\eta\hat{D}}\right) d\eta. \tag{2.5.10}$$

Let us define the *remainder* operator as

$$\hat{R}_\varepsilon = \hat{W}_\varepsilon - \hat{T}(\varepsilon), \tag{2.5.11}$$

whose operator norm can be bounded using of the previous expressions. Indeed, applying the triangular inequality, we get

$$\begin{aligned} |||\hat{R}_\varepsilon|||_2 &\leq \int_0^\varepsilon |\varepsilon - \eta| \; |||\partial_\varepsilon^2 \hat{W}_\varepsilon|||_2 \, d\eta + \int_0^\varepsilon |\varepsilon - \eta| \; |||\hat{D}^2 e^{-\mathrm{i}\varepsilon\eta\hat{D}}|||_2 d\eta \\ &\leq \int_0^\varepsilon (\varepsilon - \eta)(n+1)\gamma^2 d\eta + \int_0^\varepsilon (\varepsilon - \eta)\gamma^2 d\eta \\ &\leq \varepsilon^2\gamma^2 \left(1 + \frac{n}{2}\right), \end{aligned} \tag{2.5.12}$$

where we used that the eigenvalues of $\hat{D}$ are $\pm\gamma$ with $\gamma^2 = m^2 + ||k||_2^2$, see Subsection 2.3.1. Substituting this result into the Sobolev norm, we arrive at

$$\begin{aligned} ||W_\varepsilon\phi - T(\varepsilon)\phi||_{H^s_m} &= \sqrt{\int_{\mathbb{R}^n} (1 + m^2 + ||k||^2)^s ||\hat{R}_\varepsilon \hat{\phi}(k)||^2 \mathrm{d}k} \\ &= \sqrt{\int_{\mathbb{R}^n} (1 + m^2 + ||k||^2)^s ||\hat{R}_\varepsilon(k) \hat{\phi}(k)||^2 \mathrm{d}k} \\ &\leq \varepsilon^2 \, C \, \sqrt{\int_{\mathbb{R}^n} (1 + m^2 + ||k||^2)^{s+2} ||\hat{\phi}(k)||^2 \mathrm{d}k} \\ &\leq \varepsilon^2 \, C ||\phi||_{H^{s+2}_m}. \end{aligned} \tag{2.5.13}$$

This is what we wanted to prove, with $C = C_n = 1 + \frac{n}{2}$.

2.6 Stability

In numerical analysis, in order to evaluate the quality of a numerical scheme model, an intermediate criterion is *stability*. It demands the discrete model be a bounded linear operator. In our situation this fact is straightforward.

Proposition 2.2. *For all ϕ, for all $s \geq 0$, the equality $||W_\varepsilon\phi||_{H^s_m} = ||\phi||_{H^s_m}$ holds.*

Proof. We proceed by applying the definition of Sobolev norm, which yields

$$\begin{aligned} ||W_\varepsilon \phi||^2_{H^s_m} &= \int_{\mathbb{R}^n} (1+m^2+||k||^2)^s ||\mathcal{FT}(W_\varepsilon \phi)(k)||^2 \mathrm{d}k \\ &= \int_{\mathbb{R}^n} (1+m^2+||k||^2)^s ||(\hat{W}_\varepsilon \hat{\phi})(k)||^2 \mathrm{d}k \\ &= \int_{\mathbb{R}^n} (1+m^2+||k||^2)^s ||\hat{W}_\varepsilon(k) \hat{\phi}(k)||^2 \mathrm{d}k \end{aligned} \tag{2.6.1}$$

where in the second to third lines we used the fact that as W_ε is a translation-invariant unitary operator it is represented in Fourier space as a left multiplication by a unitary matrix $\hat{W}_\varepsilon(k)$, which depends on k. We then have

$$||W_\varepsilon \phi||^2_{H^s_m} = \int_{\mathbb{R}^n} (1+m^2+||k||^2)^s ||\hat{\phi}(k)||^2 \mathrm{d}k = ||\phi||^2_{H^s_m}. \tag{2.6.2}$$

Thus if $|||.|||_{H^s_m}$ denotes the operator norm with respect to the norm H^s_m, we have $|||W_\varepsilon|||_{H^s_m}$ equal to one, as requested. □

2.7 Convergence

In numerical analysis, in order to evaluate the quality of a numerical scheme, the most important criterion for quality is *convergence*. Intuitively it demands that, after an arbitrary time x_0, and if ε was chosen small enough, the discrete model approximates the solution to a given order of ε. Fortunately, the Lax theorem [LR56, ISEe4] states that stability and consistency implies convergence. Unfortunately, as regards the quantified version of this result, the literature available comes in many variants, with various degrees of formalization, each requesting different sets of hypotheses. Thus, for clarity, we inline the proof here.

Formally, say a Cauchy problem is well-posed on X and Y, with Y a dense subspace of X. The discrete model W_ε is convergent of order r on Y if and only if there exists C such that for any solution ψ with $\psi(x_0 = 0) \in Y$, for all $x_0 \in \mathbb{R}^+$, $l \in \mathbb{N}$, we have:

$$||W^l_{\varepsilon_l} \psi(0) - \psi(x_0)||_X = \varepsilon_l^r x_0 C ||\psi(0)||_Y \tag{2.7.1}$$

with $\varepsilon_l = x_0/l$. This is exactly what we will now prove. We state below the convergence result for the interesting case $n = 3$.

Theorem 2.1. *Let* $T(x_0) = e^{-\mathrm{i}Dx_0}$ *be the evolution operator of the free* $(3+1)$*-dimensional Dirac equation, and consider the Dirac QW:*

$$W_\varepsilon = C_\varepsilon (\mathrm{Id} \otimes H) T_{1,\varepsilon} (\mathrm{Id} \otimes HF) T_{2,\varepsilon} (\mathrm{Id} \otimes F^\dagger) T_{3,\varepsilon}.$$

Then for any solution ψ *of the Dirac equation with initial condition* $\phi \in H^{s+2}_m(\mathbb{R}^3)^4$*,* $s \geq 0$*,* *and for all $x_0 \in \mathbb{R}^+$, it holds*

$$||W_\varepsilon^l \phi - T(\varepsilon l)\phi||_{H_m^s} \leq \frac{5}{2}\varepsilon x_0 ||\phi||_{H_m^{s+2}}, \tag{2.7.2}$$

where $l = x_0/\varepsilon \in \mathbb{N}$.

2.7.1 Proof of convergence

Take $x_0 \in \mathbb{R}^+$. Consider the sequence (ε_l) such that $\varepsilon_l = x_0/l$. Because $T(\varepsilon_l l) = T(\varepsilon_l)^l$, and because

$$\sum_{j=0}^{l-1} W_{\varepsilon_l}^{l-j} T(\varepsilon_l)^j - W_{\varepsilon_l}^{l-j} T(\varepsilon_l)^j = 0 \tag{2.7.3a}$$

$$\sum_{j=0}^{l-1} W_{\varepsilon_l}^{l-j} T(\varepsilon_l)^j - W_{\varepsilon_l}^{l-j-1} T(\varepsilon_l)^{j+1} = W_{\varepsilon_l}^l - T(\varepsilon_l)^l, \tag{2.7.3b}$$

we have

$$W_{\varepsilon_l}^l \phi - T(\varepsilon_l l)\phi = \sum_{j=0}^{l-1} W_{\varepsilon_l}^{l-1-j} (W_{\varepsilon_l} - T(\varepsilon_l)) T(\varepsilon_l)^j \phi. \tag{2.7.4}$$

From consistency, there exists C such that for all ϕ,

$$||W_{\varepsilon_l} T(j\varepsilon_l)\phi - T(\varepsilon_l)T(j\varepsilon_l)\phi||_{H_m^s} \leq \varepsilon_l^2 C ||\phi||_{H_m^{s+2}}. \tag{2.7.5}$$

Hence,

$$\begin{aligned} ||W_{\varepsilon_l}^l \phi - T(\varepsilon_l l)\phi||_{H_m^s} &\leq \sum_{j=0}^{l-1} |||W_{\varepsilon_l}^{l-1-j}|||_{H_m^s} \varepsilon_l^2 C ||\phi||_{H_m^{s+2}} \\ &\leq l\varepsilon_l^2 C ||\phi||_{H_m^{s+2}} = \varepsilon_l x_0 C ||\phi||_{H_m^{s+2}}, \end{aligned} \tag{2.7.6}$$

as requested. Here $C = C_n$ is a constant only dependent on n.

2.8 Space discretization

In this chapter, we aim at giving a quantum walk model $W_\varepsilon : \ell_2(\varepsilon\mathbb{Z}^n)^d \to \ell_2(\varepsilon\mathbb{Z}^n)^d$ of the Dirac equation. So far we explained how we can discretize time in the Dirac equation, but in order to get a quantum walk, we need to discretize space as well. In a sense, this is already done since the walk operators W_ε that we defined, although they take input functions in $H^s(\mathbb{R}^n)^d$, can equally well be defined on $\ell_2(\varepsilon\mathbb{Z}^n)^d$, for the only shift operators involved in their definitions are multiples of the $T_{j,\varepsilon}$-s. The question remains, however, of what initial state we can feed our quantum walks, and how we are to interpret their output. One of the difficulties, in particular, is to construct, given $\phi \in L^2(\mathbb{R}^n)^d$, a Discretize$(\phi) \in \ell_2(\varepsilon\mathbb{Z}^n)^d$. That the discretized version of ϕ be normalized is essential so that the quantum simulation can be implemented on a quantum simulator, just like the unitarity of W_ε was essential. This section relies heavily on notations introduced in Section 2.3.

The main result of this section is the following.

Theorem 2.2. *For a discretization parameter ε, a number of iterations l, and if $x_0 = \varepsilon l$ is the total evolution time, then the overall error is*

$$\|\textit{Reconstruct}(W_\varepsilon^l(\textit{Discretize}(\phi))) - T(\varepsilon l)\phi\|_{H_m^s} \leq \varepsilon^2 C||\phi||_{H_m^{s+2}}, \tag{2.8.1}$$

for some constant $C > 0$ which only depends on l and the dimensions n.

The proof is organized in three steps. In 2.8.1, we formalize the discretization procedure. In 2.8.2-2.8.3. Then, the overall bound is computed in 2.8.4.

2.8.1 Discretization procedure

We discretize by

$$\text{Discretize}(\phi) = \text{Renormalize}(\mathcal{FS}(\mathcal{FT}(\phi)|_{[-\frac{\pi}{\varepsilon},\frac{\pi}{\varepsilon}]^n})). \tag{2.8.2}$$

Notice that

$$\phi_{\text{LP}} = \mathcal{FT}^{-1}(\chi_{[-\frac{\pi}{\varepsilon},\frac{\pi}{\varepsilon}]^n}\mathcal{FT}(\phi)), \tag{2.8.3}$$

where χ_A denotes the indicator function of A, applies an ideal low-pass filter, and that

$$\mathcal{FS}(\mathcal{FT}(\phi_{\text{LP}})|_{[-\frac{\pi}{\varepsilon},\frac{\pi}{\varepsilon}]^n}) = \varepsilon^{n/2}\phi_{\text{LP}}|_{\varepsilon\mathbb{Z}^n} \tag{2.8.4}$$

is, up to a constant, the sampling of ϕ_{LP}, see Subsection 2.3.2. Discretize(ϕ) is hence proportional to the function obtained by sampling ϕ after it has been low-pass filtered. Since $\mathcal{FS}$ and $\mathcal{FT}$ are unitary, the renormalization is by a factor of $\|\phi_{\text{LP}}\|_2^{-1}$. For it to be well-defined, we must check that ϕ_{LP} does have a non-zero norm.

2.8.2 Low-pass filtering

For every $s \geq 0$, we have

$$\begin{aligned}
\|\phi - \phi_{\text{LP}}\|_{H_m^s}^2 &= \int_{\mathbb{R}^n\setminus[-\frac{\pi}{\varepsilon},\frac{\pi}{\varepsilon}]^n} (1 + m^2 + \|k\|^2)^s \|\hat{\phi}(k)\|^2 \mathrm{d}k \\
&= \int_{\mathbb{R}^n\setminus[-\frac{\pi}{\varepsilon},\frac{\pi}{\varepsilon}]^n} (1 + m^2 + \|k\|^2)^{-2}(1 + m^2 + \|k\|^2)^{s+2} \|\hat{\phi}(k)\|^2 \mathrm{d}k \\
&\leq \left(\varepsilon^2 C' \|\phi\|_{H_m^{s+2}}\right)^2 \quad \text{with} \quad C' = \pi^{-2}.
\end{aligned} \tag{2.8.5}$$

This tells us two things. First, if $\varepsilon^2 < \frac{\|\phi\|_2}{C'\|\phi\|_{H_m^2}}$, then $\phi_{\text{LP}} \neq 0$, so it can be renormalized. Second, the loss induced by low-pass filtering is small, as needed below in order to bound the overall error.

2.8.3 Reconstruction procedure

We reconstruct by

$$\text{Reconstruct}(\tilde{\phi}) = \mathcal{FT}^{-1}(\mathcal{FS}^{-1}(\text{Renormalize}^{-1}(\tilde{\phi}))), \tag{2.8.6}$$

with the convention that $\mathcal{FS}^{-1}(\tilde{\phi}) \in L^2([-\frac{\pi}{\varepsilon}, \frac{\pi}{\varepsilon}]^n)^d$ is extended to $L^2(\mathbb{R}^n)^d$ by the null function on $\mathbb{R}^n \setminus [-\frac{\pi}{\varepsilon}, \frac{\pi}{\varepsilon}]^n$, and the inverse renormalization is by a factor of $\|\phi_{\text{LP}}\|_2$. Notice that $\phi_{\text{LP}} = \text{Reconstruct}(\text{Discretize}(\phi_{\text{LP}}))$, and that this reconstruction is equivalent to the Whittaker-Kotelnikov-Shannon formula (cf. [PM62], [JG04] for the multidimensional case).

2.8.4 Overall scheme

Given a wave function ϕ, we approximate $T(\varepsilon l)\phi$, the continuous evolution of ϕ, by

$$\text{Reconstruct}(W_\varepsilon^l(\text{Discretize}(\phi))), \tag{2.8.7}$$

the reconstruction of the walk iterated on the discretization of ϕ. Let us bound the overall error. For all ϕ we have (renormalizations cancel out by linearity of W_ε^l):

$$\begin{aligned}
\text{Reconstruct}(W_\varepsilon^l(\text{Discretize}(\phi))) &= \mathcal{FT}^{-1}(\mathcal{FS}^{-1}(W_\varepsilon^l(\mathcal{FS}(\mathcal{FT}(\phi)|_{[-\frac{\pi}{\varepsilon},\frac{\pi}{\varepsilon}]^n})))) \\
&= \mathcal{FT}^{-1}(\mathcal{FS}^{-1}(W_\varepsilon^l(\mathcal{FS}(\mathcal{FT}(\phi_{\text{LP}}))))) \\
&= \mathcal{FT}^{-1}(\mathcal{FS}^{-1}(W_\varepsilon^l(\varepsilon^{n/2}\phi_{\text{LP}}|_{\varepsilon\mathbb{Z}^n}))) \\
&= \mathcal{FT}^{-1}(\mathcal{FS}^{-1}(\varepsilon^{n/2}W_\varepsilon^l(\phi_{\text{LP}})|_{\varepsilon\mathbb{Z}^n})) \\
&= \mathcal{FT}^{-1}(\mathcal{FT}(W_\varepsilon^l(\phi_{\text{LP}}))|_{[-\frac{\pi}{\varepsilon},\frac{\pi}{\varepsilon}]^n}) \\
&= W_\varepsilon^l(\phi_{\text{LP}})
\end{aligned} \tag{2.8.8}$$

where the preceding step comes from (2.3.10). Now, since W_ε^l is unitary, we have

$$\|W_\varepsilon^l(\phi_{\text{LP}}) - W_\varepsilon^l(\phi)\|_{H_m^s} = \|\phi_{\text{LP}} - \phi\|_{H_m^s} \leq \varepsilon^2 C' \|\phi\|_{H_m^{s+2}}. \tag{2.8.9}$$

On the other hand in Section 2.7 we had:

$$\|W_\varepsilon^l(\phi) - T(\varepsilon l)(\phi)\|_{H_m^s} \leq \varepsilon^2 lC||\phi||_{H_m^{s+2}}. \tag{2.8.10}$$

And thus the bound on the overall error is:

$$\|\text{Reconstruct}(W_\varepsilon^l(\text{Discretize}(\phi))) - T(\varepsilon l)\phi\|_{H_m^s} \leq \varepsilon^2(lC + C')||\phi||_{H_m^{s+2}}. \tag{2.8.11}$$

where in the last inequality we should recall that ε is the discretization parameter and l the number of iterations, thus $x_0 = \varepsilon l$ is for how long the evolution is simulated.

2.9 Summary

Nowadays, simulation of physical processes is realized over classical computers, and the quality of the result is validated by numerical analysis. With the future development of quantum computers, the quantum simulation of physical processes will also need to be validated. Based on simple arguments, our approach allows to obtain convergence of the solutions from stability and consistency, without ever having to obtain the solutions themselves. This is a key point: this method will apply equally well to more complicated QWs, e.g. in principle could be applied to Bargmann-Wigner equations describing arbitrary spin relativistic wave equations, or even symmetric hyperbolic systems in general.

The QW is parametrized on ε, the discretization step. It is of course tempting to set ε to in Planck units, and grant

$$W = C(\mathrm{Id} \otimes H)T_1(\mathrm{Id} \otimes HF)T_2(\mathrm{Id} \otimes F^\dagger)T_3 \tag{2.9.1}$$

a more fundamental status. One could even wonder whether some relativistic particles might behave according to this QW, rather than the Dirac equation. For setting this idea on stronger grounds, the next chapter points in one of these possible directions. We study to which extent such discrete models retain Lorentz covariance.

Chapter 3

Discrete Lorentz covariance

We have seen that QWs are dynamics whose main features are being: discrete in time and space (i.e. a unitary evolution of the wave-function of a particle on a lattice); homogeneous (i.e. translation-invariant and time-independent), and causal (i.e. information propagates at a bounded speed, in a strict sense). Therefore, they have several of the fundamental symmetries of physics, built-in. But can they also have Lorentz covariance? In this chapter, we give a positive answer, by formalizing a notion of discrete Lorentz transforms for QWs and QCAs. Already in the reduced $(1+1)$-dimensional discrete spacetime there are several difficulties that need to be overcome, and all the chapter is placed in this setting. The theory admits a diagrammatic representation in terms of a few local, circuit equivalence rules. Within this framework, we show the first-order-only covariance of the Dirac QW. We then introduce the Clock QW and the Clock QCA, and prove that they are exactly discrete Lorentz covariant. The theory also allows for non-homogeneous Lorentz transforms between non-inertial frames.

This chapter is organized as follows. We start in Section 3.1 stating our approach, the notations, and recalling the proof of covariance of the Dirac equation. In Section 3.2 we discuss the first-order-only covariance of the Dirac QW. In Section 3.3 we formalize discrete Lorentz transforms, covariance, and discuss non-homogeneous Lorentz transforms. In Sections 3.4 and 3.5 apply this theory to the Clock QW and the Clock QCA respectively. We finish with a discussion of the physical interpretation in Section 3.6, and summarize our results in Section 3.7.

3.1 Introduction

In this chapter we formalize a notion of discrete Lorentz transforms, acting upon wave-functions over discrete spacetime. It formalizes the notion of discrete Lorentz covariance of a QW, by demanding that a solution of the QW be Lorentz transformed into another solution, of the same QW. Our approach is non-statistical: we look for exact Lorentz covariance. Spacetime remains undeformed, always assumed to be a regular lattice, and the QW remains homogeneous. While keeping to $1+1$ dimensions and integral transforms, we allow for a global rescaling, so that we can represent all Lorentz transforms with rational velocity. The basic idea is to map each point of the lattice to a lightlike rectangular spacetime patch, as illustrated in Figs. 3.1.1 and 3.3.4.

Before the formalism is introduced, we investigate a concrete example: the Dirac QW [SB93, BB94, Mey96, ANF14]. The Dirac QW is a natural candidate for being Lorentz covariant, because its continuum limit is the covariant, free-particle Dirac equation [Str07, ANF14, BDT13]. This example helps us build our definitions. However, the Dirac QW turns out to be first-order covariant only. In order to obtain exact Lorentz covariance, we introduce a new model, the Clock QW, which arises as the quantum version of a covariant classical Random Walk [Wal88]. However, the Clock QW requires an observer-dependent dimension for the internal state space. In order to overcome this problem, the formalism is extended to multiple-walkers QWs, i.e. Quantum Cellular Automata (QCA). Indeed, the Clock QCA provides a first finite-dimensional model of an exactly covariant QCA. We use numerous figures to help our intuition. In fact, the theory admits a simple diagrammatic representation, in terms of a few local, circuit equivalence rules. The theory also allows for non-homogeneous Lorentz transforms, a specific class of general coordinate transformations, and yet expressive enough to switch between non-inertial frames.

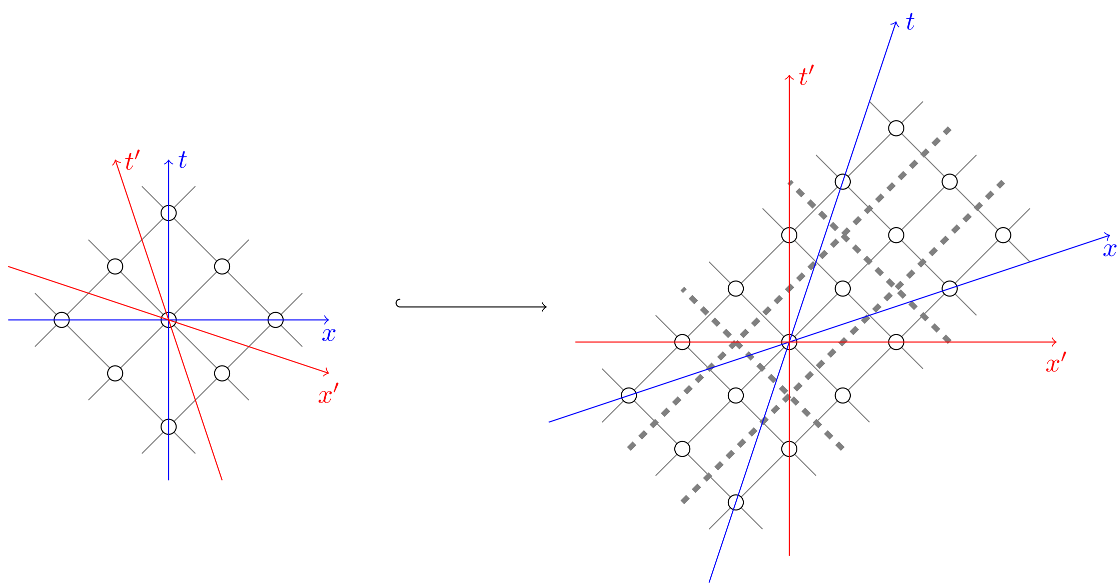
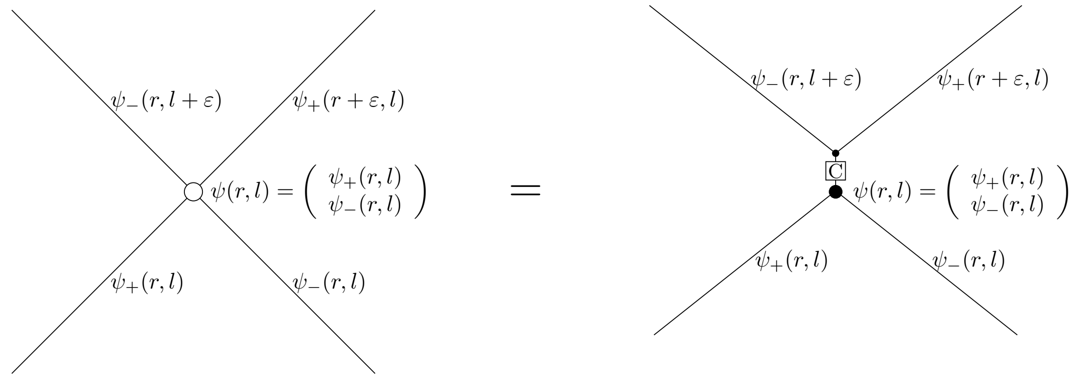


Figure 3.1.1: *Conceptual diagram for the discrete Lorentz transform.* In this example $\alpha = 2$, $\beta = 1$. Each point in the original reference frame is transformed into a lightlike rectangular spacetime patch of $\alpha \times \beta$ points, here enclosed by the dashed lines. This switches from the x, t frame to the x', t' frame, as shown.

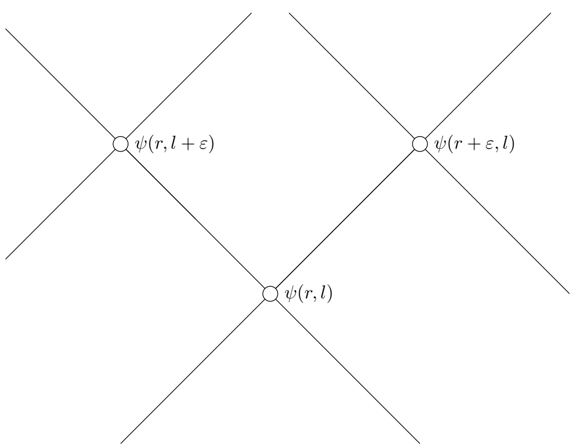
3.1.1 Finite Difference Dirac Eq. and the Dirac QW

The Dirac Equation. The (1+1)-dimensional free particle Dirac equation is (with Planck's constant and the velocity of light set to one):

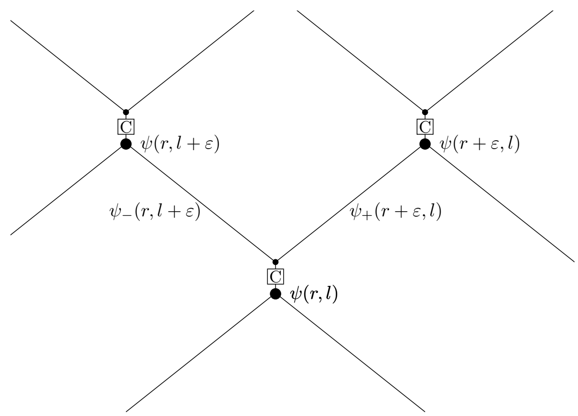
$$\partial_t \psi = -\mathrm{i} m \sigma_1 \psi - \partial_x \sigma_3 \psi, \tag{3.1.1}$$



(a) Each white dot (left) represents the corresponding piece of circuit (right).



(b) A discrete spacetime wavefunction ψ in lightlike coordinates. Time flows upwards.



(c) An explicit circuit-like representation of the relationship between the vectors at each point. The matrix C gets applied upon its input vector, whereas each lightlike wire propagates just one scalar component of the output vector.

Figure 3.1.2: *Discrete spacetime wavefunctions that are solutions of the FD Dirac or the Dirac QW.*

where m is the mass of the particle, $\psi = \psi(t,x)$ is a spacetime wavefunction from $\mathbb{R}^{1+1}$ to $\mathbb{C}^2$ and σ_j ($j = 0, \ldots, 3$) are the Pauli spin matrices, with σ_0 the identity. Eq. (3.1.1) corresponds to the Weyl (or spinor) representation [Tha92].

Lightlike coordinates. In order to study covariance, it is always a good idea to switch to lightlike coordinates $r = (t+x)/2$ and $l = (t-x)/2$, in which a Lorentz transform is just a rescaling of the coordinates. Redefine the wavefunction via $\psi(r+l, r-l) \to \psi(r,l)$, then Eq. (3.1.1) becomes

$$\mathrm{diag}\partial_r\partial_l\psi = -\mathrm{i}m\sigma_1\psi. \tag{3.1.2}$$

Finite-difference Dirac Equation. In this chapter $e^{\varepsilon\partial_\mu}$ will be used as a notation for the translation by ε along the μ-axis (with $\mu = 0,1$), i.e. $(e^{\varepsilon\partial_\mu}\psi)(x_\mu) = \psi(x_\mu + \varepsilon)$.

Using the first order expansion of the the exponential, the spacetime wavefunction ψ is a solution of the Dirac equation if and only if, as $\varepsilon \to 0$,

$$\begin{aligned} \mathrm{diag} e^{\varepsilon\partial_r} e^{\varepsilon\partial_l}\psi &= (\mathrm{Id} + \mathrm{diag}\varepsilon\partial_r\varepsilon\partial_l)\,\psi + O(\varepsilon^2) \\ &= (\mathrm{Id} - \mathrm{i}m\varepsilon\sigma_1)\psi + O(\varepsilon^2). \end{aligned} \tag{3.1.3}$$

Equivalently, if we denote $\psi = (\psi_+, \psi_-)^\mathsf{T}$, then ψ is a solution of the Dirac equation if and only if, to first order in ε and as $\varepsilon \to 0$,

$$\begin{aligned} &\psi_+(r+\varepsilon, l) = \psi_+(r,l) - \mathrm{i}m\varepsilon\psi_-(r,l) \\ \text{and} \quad &\psi_-(r, l+\varepsilon) = \psi_-(r,l) - \mathrm{i}m\varepsilon\psi_+(r,l). \end{aligned} \tag{3.1.4}$$

If we now suppose that ε is fixed, and consider that ψ is a spacetime wavefunction from $(\varepsilon\mathbb{Z})^2$ to $\mathbb{C}^2$, then Eq. (3.1.4) defines a Finite-difference scheme for the Dirac equation (FD Dirac). As a dynamical system, this FD Dirac is illustrated in Fig. 3.1.2 with:

$$C = \begin{pmatrix} 1 & -\mathrm{i}\varepsilon m \\ -\mathrm{i}\varepsilon m & 1 \end{pmatrix}. \tag{3.1.5}$$

The Dirac QW. We could have gone a little further with Eq. (3.1.3). Indeed, by recognizing in the right-hand side of the equation the first order expansion of an exponential, we get:

$$\mathrm{diag} e^{\varepsilon\partial_r} e^{\varepsilon\partial_l}\psi = e^{-\mathrm{i}m\varepsilon\sigma_1}\psi + O(\varepsilon^2). \tag{3.1.6}$$

In fact, ψ is a solution of the Dirac equation if and only if, as $\varepsilon \to 0$, Eq. (3.1.6) is satisfied. See [Str07, ANF14] for a rigorous, quantified proof of convergence.

If we again say that ε is fixed, and so that ψ is a discrete spacetime wavefunction, then Eq. (3.1.6) defines a Quantum Walk for the Dirac equation (Dirac QW) [SB93, BB94, Mey96, BDT13, ANF14]. Indeed, as a dynamical system, this Dirac QW is again illustrated in Fig. 3.1.2 but this time taking:

$$C = e^{-\mathrm{i}m\varepsilon\sigma_1} = \begin{pmatrix} \cos(\varepsilon m) & -\mathrm{i}\sin(\varepsilon m) \\ -\mathrm{i}\sin(\varepsilon m) & \cos(\varepsilon m) \end{pmatrix}, \tag{3.1.7}$$

which is exactly unitary, i.e. to all orders in ε.

In the original (t, x) coordinates, both the FD Dirac and the Dirac QW evolutions are given by $\psi(t+\varepsilon, x) = TC\psi(t,x)$, where $T = e^{-\varepsilon\partial_x\sigma_3}$ is the shift operator and C is the matrix appearing in Eq. (3.1.5) or Eq. (3.1.7) respectively (see [ANF14] for details). In the case of the Dirac QW, $W = TC$ is referred to as the walk operator: it is shift-invariant and unitary. C is referred to as the coin operator, acting over the ‘coin space’, which is $\mathcal{H} \cong \mathbb{C}^2$ for the Dirac QW. Eq. (3.1.6) reads as follows: the top and bottom components of the coin space get mixed up by the coin operator, and then the top component moves at lightspeed towards the right, whereas the bottom component goes in the opposite direction.

Remark 3.1. Let α, β be arbitrary positive integers. Notice that knowing the value of the scalars $\psi_-(r,l),\dots,\psi_-(r+(\alpha-1)\varepsilon,l)$ carried by the right-incoming wires, together with the scalars $\psi_+(r,l),\dots,\psi_+(r,l+(\beta-1)\varepsilon)$ carried by the left-incoming wires, fully determines $\psi(r+i\varepsilon,l+j\varepsilon)$ for $0\le i\le(\alpha-1)$ and $0\le j\le(\beta-1)$, as made apparent in Fig. 3.1.3. We denote by $\overline{C}(i,j)$ the operator which, given the vectors

$$\overline{\psi}_-(r,l)=\begin{pmatrix}\psi_-(r,l)\\ \vdots\\ \psi_-(r+(\alpha-1)\varepsilon,l)\end{pmatrix}$$

and

$$\overline{\psi}_+(r,l)=\begin{pmatrix}\psi_+(r,l)\\ \vdots\\ \psi_+(r,l+(\beta-1)\varepsilon)\end{pmatrix}$$

combined as

$$\overline{\psi}(r,l)=\begin{pmatrix}\overline{\psi}_+(r,l)\\ \overline{\psi}_-(r,l)\end{pmatrix},$$

yields $\psi(r+i\varepsilon,l+j\varepsilon)$, i.e. $\psi(r+i\varepsilon,l+j\varepsilon)=\overline{C}(i,j)\overline{\psi}(r,l)$. Moreover, notice that those values also determine the right outcoming wires $\psi_+(r+\alpha\varepsilon,l+j\varepsilon)$ for $0\le j\le(\beta-1)$, which we denote by $\overline{C}_+\overline{\psi}(r,l)$, and the left outcoming wires $\psi_-(r+i\varepsilon,l+\beta\varepsilon)$ for $0\le i\le(\alpha-1)$, which we denote be $\overline{C}_-\overline{\psi}(r,l)$. More generally, we denote by $\overline{C}$ the circuit made of $(\alpha\beta)$ gates shown in Fig. 3.1.3, i.e.

$$\overline{C}\,\overline{\psi}(r,l)=\left(\overline{C}_+\oplus\overline{C}_-\right)\overline{\psi}(r,l). \tag{3.1.8}$$

We write $\overline{C}_m$ for the operator, instead of $\overline{C}$, when we want to make explicit its dependency upon the parameter m.

3.1.2 Scaled Lorentz transforms and covariance

Let us review the covariance of the Dirac equation in a simple manner, that will be useful for us later. Consider a change of coordinates $r'=\alpha r$, $l'=\beta l$. This transformation is proportional by a factor of $\sqrt{\alpha\beta}$ to the Lorentz transform

$$\Lambda=\begin{pmatrix}\sqrt{\dfrac{\alpha}{\beta}} & 0\\ 0 & \sqrt{\dfrac{\beta}{\alpha}}\end{pmatrix} \tag{3.1.9}$$

whose velocity parameter is $u=(\alpha-\beta)/(\alpha+\beta)$. Let us define $\widetilde{\psi}(r',l')=\widetilde{\psi}(\alpha r,\beta l)=\psi(r,l)$. A translation by ε along r (resp. l) becomes a translation by $\alpha\varepsilon$ along r' (resp. $\beta\varepsilon$

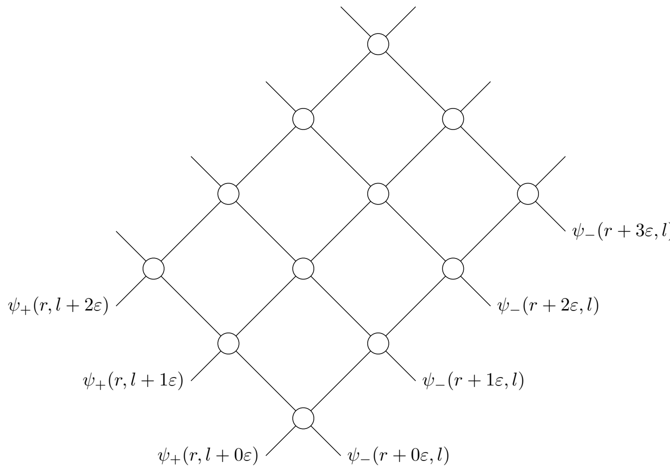


Figure 3.1.3: *Lightlike rectangular patches of spacetime* (in this example $\alpha = 4$, $\beta = 3$) are fully-determined by the incoming wires.

along l'). Hence the Dirac equation now demands that as $\varepsilon \to 0$,

$$\mathrm{diag} e^{\alpha\varepsilon\partial_{r'}} e^{\beta\varepsilon\partial_{l'}} \widetilde{\psi} = \begin{pmatrix} 1 & -\mathrm{i}\varepsilon m \\ -\mathrm{i}\varepsilon m & 1 \end{pmatrix} \widetilde{\psi} + O(\varepsilon^2). \tag{3.1.10}$$

Equivalently, to first order in ε and as $\varepsilon \to 0$,

$$\widetilde{\psi}_+(r' + \alpha\varepsilon, l') = \widetilde{\psi}_+(r', l') - \mathrm{i}m\varepsilon\widetilde{\psi}_-(r', l') \tag{3.1.11a}$$

$$\widetilde{\psi}_-(r', l' + \beta\varepsilon) = \widetilde{\psi}_-(r', l') - \mathrm{i}m\varepsilon\widetilde{\psi}_+(r', l') \tag{3.1.11b}$$

Unfortunately, whenever $\alpha \neq \beta$, this is not in the form of a Dirac equation. In other words the coordinate change alone does not take the Dirac equation into the Dirac equation.

Remark 3.2. In Section 3.4 we will study the Clock QW, inspired by:

$$\begin{pmatrix} e^{\alpha\varepsilon\partial_r} & 0 \\ 0 & e^{\beta\varepsilon\partial_l} \end{pmatrix} \psi = e^{-\mathrm{i}m\varepsilon\sigma_1}\psi. \tag{3.1.12}$$

Meanwhile, notice that in the first order, the top and bottom ε can be taken to be different, leading to

$$\mathrm{diag} e^{\varepsilon\partial_{r'}} e^{\varepsilon\partial_{l'}} \widetilde{\psi} = \begin{pmatrix} 1 & -\mathrm{i}\varepsilon m/\alpha \\ -\mathrm{i}\varepsilon m/\beta & 1 \end{pmatrix} \widetilde{\psi} + O(\varepsilon^2). \tag{3.1.13}$$

$$\mathrm{diag} e^{\varepsilon\partial_{r'}} e^{\varepsilon\partial_{l'}} \begin{pmatrix} \widetilde{\psi}_+/\sqrt{\beta} \\ \widetilde{\psi}_-/\sqrt{\alpha} \end{pmatrix} =$$
$$\begin{pmatrix} 1 & -\mathrm{i}\varepsilon m/\sqrt{\alpha\beta} \\ -\mathrm{i}\varepsilon m/\sqrt{\alpha\beta} & 1 \end{pmatrix} \begin{pmatrix} \widetilde{\psi}_+/\sqrt{\beta} \\ \widetilde{\psi}_-/\sqrt{\alpha} \end{pmatrix} + O(\varepsilon^2). \qquad (3.1.14)$$

Let us define

$$S = \begin{pmatrix} 1/\sqrt{\beta} & 0 \\ 0 & 1/\sqrt{\alpha} \end{pmatrix} \qquad \text{and} \qquad \psi' = S\widetilde{\psi}. \qquad (3.1.15)$$

Call this ψ' the Lorentz transformed of ψ, instead of $\widetilde{\psi}$. Now we have:

$$\mathrm{diag} e^{\varepsilon\partial_{r'}} e^{\varepsilon\partial_{l'}} \psi' = \begin{pmatrix} 1 & -\mathrm{i}\varepsilon m/\sqrt{\alpha\beta} \\ -\mathrm{i}\varepsilon m/\sqrt{\alpha\beta} & 1 \end{pmatrix} \psi' \qquad (3.1.16)$$

i.e. the Dirac equation just for a different mass $m' = m/\sqrt{\alpha\beta}$. This different mass is due to the fact that the transformation to primed coordinates that we considered was a scaled Lorentz transform. In the special case where $\alpha\beta = 1$, the above is just the proof of Lorentz covariance of the Dirac equation.

3.2 A discrete Lorentz transform for the Dirac QW

3.2.1 Normalization problem and its solution

Normalization problem in the discrete case. Take $\psi(r, l)$ a solution of the Dirac QW such that the initial condition is normalized and localized at single point e.g. $\psi(0, 0) = (1, 0)^\mathsf{T}$ and $\psi(r, l) = (0, 0)^\mathsf{T}$ for $t = r + l = 0$. Then, after applying the Lorentz transform described in Subsection 3.1.2, the initial condition is $\psi'(0, 0) = (1/\sqrt{\beta}, 0)^\mathsf{T}$ and $\psi'(r, l) = (0, 0)^\mathsf{T}$ for $t = r + l = 0$ which is not normalized for any non-trivial Lorentz transform, see Fig. 3.2.1(a). Hence, we see that the Lorentz transform described in Subsection 3.1.2, i.e. that used for the covariance of the continuous Dirac equation, is problematic in the discrete case: the transformed observer sees a wavefunction which is not normalized. This seems a paradoxical situation since in the limit when $\varepsilon \to 0$, the discrete case tends towards the continuous case, which does not have such a normalization issue. In order to fix this problem, let us look more closely at how normalization is preserved in the continuous case.

Normalization in the continuous case. Now take $\psi(r, l)$ a solution of the massless Dirac equation such that the initial condition is the normalized, right-moving rectangular function, i.e. $\psi(r, l) = (1/\sqrt{2}, 0)^\mathsf{T}$, for $0 \leq l < 1$ and $\psi(r, l) = (0, 0)^\mathsf{T}$ elsewhere. The Lorentz transform of ψ is

$$\psi'(r', l') = S\psi(r'/\alpha, l'/\beta) = \begin{cases} \begin{pmatrix} 1/\sqrt{2\beta} \\ 0 \end{pmatrix} & 0 \leq l' < \beta \\ \begin{pmatrix} 0 \\ 0 \end{pmatrix} & \text{elsewhere,} \end{cases} \qquad (3.2.1)$$

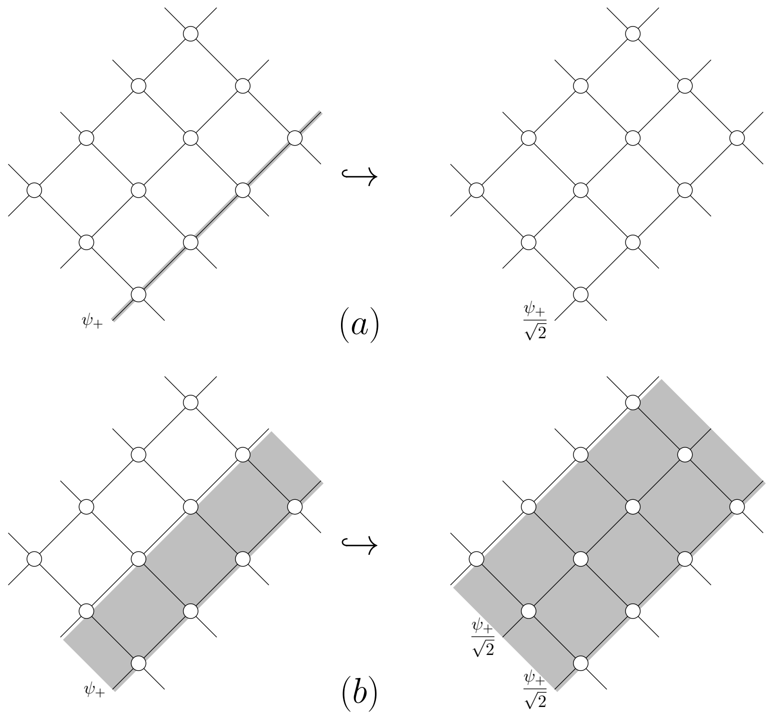


Figure 3.2.1: *The normalization problem and solution in the* $m = 0$*,* $\alpha = 1$*,* $\beta = 2$ *case.* (a) If $\psi_+(0,0)$ gets interpreted as a right-traveling Dirac peak, then its transformed version is $\psi'_+(0,0) = \psi_+(0,0)/\sqrt{2}$, which is not normalized. (b) If $\psi_+(0,0)$ gets interpreted as a right-moving rectangular function, then its transformed version spreads out as $\psi'_+(0,0) = \psi'_+(0,1) = \psi_+(0,0)/\sqrt{2}$, which is normalized.

which is normalized. We see that the S matrix is no longer a problem for normalization, but rather it is needed to compensate for the larger spread of the wavefunction, see Fig. 3.2.1(b). This suggests that the normalization problem for the localized initial condition in the discrete case could be fixed, by allowing the discrete Lorentz transform to spread out the initial condition.

From the continuous to the discrete. Intuitively, we could think of defining the discrete Lorentz transform as the missing arrow "Discrete Λ?" that would make the following diagram commute:

$$\begin{array}{ccc} \text{Dirac} & \xrightarrow{\Lambda} & \text{Dirac}' \\ \big\downarrow{\scriptstyle \text{Discretize}} & & \big\downarrow{\scriptstyle \text{Discretize}} \\ \text{QW} & \xrightarrow{\text{Discrete } \Lambda?} & \text{QW}' \end{array} \tag{3.2.2}$$

In other words,

$$\text{Discrete } \Lambda \circ \text{Discretize} := \text{Discretize} \circ \Lambda \tag{3.2.3}$$

and hence,

$$\text{Discrete }\Lambda := \text{Discretize} \circ \Lambda \circ \text{Interpolate} \tag{3.2.4}$$

For instance, if the localized walker was to be interpolated as a rectangular function instead of a Dirac peak, that rectangular function will be spread out by the continuous Λ, and may discretize as a more spread out walker. The discrete Lorentz transform that we propose next does just that. However, it will be phrased directly in the discrete setting. Later in Section 3.3 we provide a more general and diagrammatic definition of discrete Lorentz transform and discrete Lorentz covariance.

3.2.2 A discrete Lorentz transform

In the continuous case we had $\psi'(r',l') = S\psi(r,l)$. Hence $\psi'(r',l') = S\psi(r'/\alpha, l'/\beta)$. In the discrete case, however ψ is a spacetime wavefunction from $(\varepsilon\mathbb{Z})^2$ to $\mathbb{C}^2$, as in Fig. 3.1.2(b). Hence, demanding, for instance, that $\psi'(\varepsilon,0) = S\psi(\varepsilon/\alpha,0)$ becomes meaningless, because $\psi(\varepsilon/\alpha,0)$ is undefined. The normalization issues and the related discussion of Subsection 3.2.1 suggests setting $\psi'_-(\varepsilon,0)$ to $S\psi_-(0,0)$, and not to 0. More generally, we will take:

$$\forall r' \in \varepsilon\alpha\mathbb{Z}, \quad \psi'_+(r',l') = \frac{\psi_+(r'/\alpha, \lfloor l'/\beta \rfloor_\varepsilon)}{\sqrt{\beta}} \tag{3.2.5}$$

and

$$\forall l' \in \varepsilon\beta\mathbb{Z}, \quad \psi'_-(r',l') = \frac{\psi_-(\lfloor r'/\alpha \rfloor_\varepsilon, l'/\beta)}{\sqrt{\alpha}}. \tag{3.2.6}$$

where $\lfloor . \rfloor_\varepsilon$ takes the closest multiple of ε that is less or equal to the number. Notice that this implies that for all $r' \in \varepsilon\alpha\mathbb{Z}$ and $l' \in \varepsilon\beta\mathbb{Z}$, we have $\psi'(r',l') = S\psi(r'/\alpha, l'/\beta)$, as in the continuous case. However, what if we have neither $r' \in \alpha\varepsilon\mathbb{Z}$ nor $l' \in \beta\varepsilon\mathbb{Z}$? As was illustrated in Fig. 3.1.3, this spacetime region is now fully determined, i.e. we set

$$\forall r', l' \in \varepsilon\mathbb{Z}, \quad \psi'(r',l') = \overline{C}_{m'}(i,j)\overline{\psi'}(\lfloor r' \rfloor_{\alpha\varepsilon}, \lfloor l' \rfloor_{\beta\varepsilon}) \tag{3.2.7}$$

with $m' = m/\sqrt{\alpha\beta}$, $i\varepsilon = r' - \lfloor r' \rfloor_{\alpha\varepsilon}$, $j\varepsilon = l' - \lfloor l' \rfloor_{\beta\varepsilon}$, $\overline{C}_{m'}(i,j)$ as defined in Remark 3.1, and $\overline{\psi'}(\lfloor r' \rfloor_{\alpha\varepsilon}, \lfloor l' \rfloor_{\beta\varepsilon})$ again as defined in Remark 3.1, namely

$$\begin{aligned}
\overline{\psi'}_+(\lfloor r' \rfloor_{\alpha\varepsilon}, \lfloor l' \rfloor_{\beta\varepsilon}) &= \begin{pmatrix} \psi'_+(\lfloor r' \rfloor_{\alpha\varepsilon}, \lfloor l' \rfloor_{\beta\varepsilon}) \\ \vdots \\ \psi'_+(\lfloor r' \rfloor_{\alpha\varepsilon}, \lfloor l' \rfloor_{\beta\varepsilon} + (\beta-1)\varepsilon) \end{pmatrix} \\
&= \begin{pmatrix} \dfrac{\psi_+(\lfloor r' \rfloor_{\alpha\varepsilon}, \lfloor l' \rfloor_{\beta\varepsilon})}{\sqrt{\beta}} \\ \vdots \end{pmatrix}
\end{aligned}$$

and similarly

$$\overline{\psi'}_{-}(\lfloor r' \rfloor_{\alpha\varepsilon}, \lfloor l' \rfloor_{\beta\varepsilon}) = \begin{pmatrix} \frac{\psi_{-}(\lfloor r' \rfloor_{\alpha\varepsilon}, \lfloor l' \rfloor_{\beta\varepsilon})}{\sqrt{\alpha}} \\ \vdots \end{pmatrix}$$

and finally

$$\overline{\psi'}(\lfloor r' \rfloor_{\alpha\varepsilon}, \lfloor l' \rfloor_{\beta\varepsilon}) = \begin{pmatrix} \overline{\psi'}_{+}(\lfloor r' \rfloor_{\alpha\varepsilon}, \lfloor l' \rfloor_{\beta\varepsilon}) \\ \overline{\psi'}_{-}(\lfloor r' \rfloor_{\alpha\varepsilon}, \lfloor l' \rfloor_{\beta\varepsilon}) \end{pmatrix}.$$

This finishes to define a discrete Lorentz transform $L_{\alpha,\beta}$, which is illustrated in Fig. 3.2.2.

An equivalent, more concise way of specifying this discrete Lorentz transform $L_{\alpha,\beta}$ is as follows. First, consider the isometry E_β (resp. E_α) which codes $\psi_+(r,l)$ (resp. $\psi_-(r,l)$) into the more spread out $\breve{\psi}_+(r,l) = E_\beta\psi_+(r,l) = \overline{\psi'}_+(\alpha r, \beta l)$ (resp. $\breve{\psi}_-(r,l) = E_\alpha\psi_-(r,l) = \overline{\psi'}_-(\alpha r, \beta l)$), and let $\breve{\psi}(r,l) = \breve{\psi}_+(r,l) \oplus \breve{\psi}_-(r,l)$, and $m' = m/\sqrt{\alpha\beta}$. Second, construct $\psi' = L_{\alpha,\beta}\psi$ by replacing every spacetime point $\psi(r,l)$ with the lightlike rectangular spacetime patch $\left(\overline{C}_{m'}(i,j)\breve{\psi}(r,l)\right)_{i=0\ldots(\alpha-1), j=0\ldots(\beta-1)}$.

Does this discrete Lorentz transform fix the normalization problem of Subsection 3.2.1? Let us evaluate this question.

3.2.3 From continuous to discrete current and norm

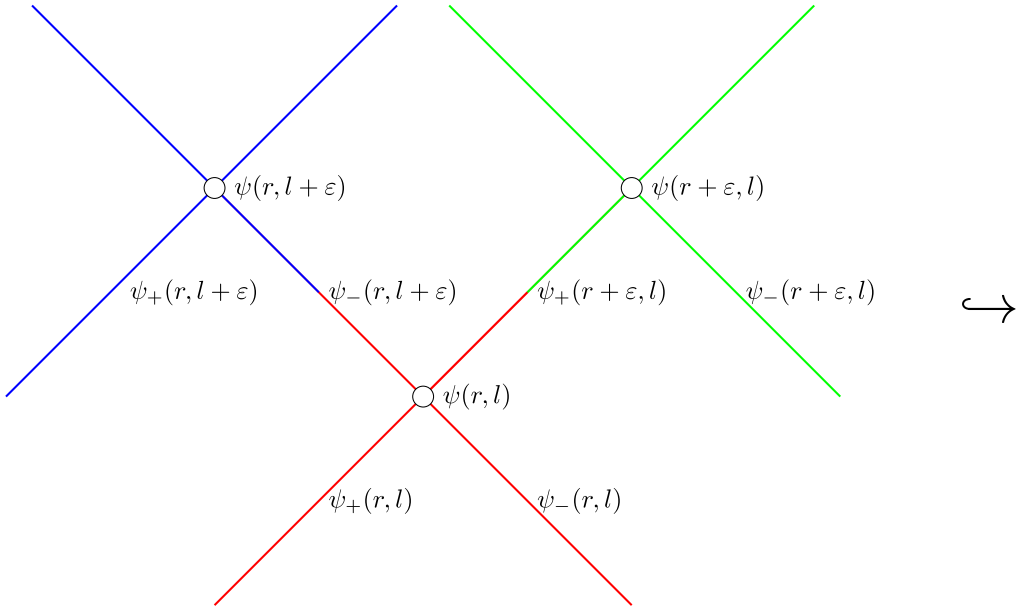
3.2.3.1 Continuous current and norm

In order to evaluate the norm of a spacetime wavefunction ψ in the continuous setting, we need the following definition. We say that a surface σ is a *Cauchy surface* if it intersects every causal curve exactly once (a causal curve being a curve whose tangent vector is always timelike or lightlike). The relativistic current $j^\mu = (j^0, j^1)$ is equal to $j^\mu = (|\psi_+|^2 + |\psi_-|^2, |\psi_+|^2 - |\psi_-|^2)$, and in lightlike coordinates becomes $j^s = (|\psi_+|^2, |\psi_-|^2)$, $s = \pm$. The norm of ψ along a Cauchy surface σ is defined by integrating the current j^s along σ

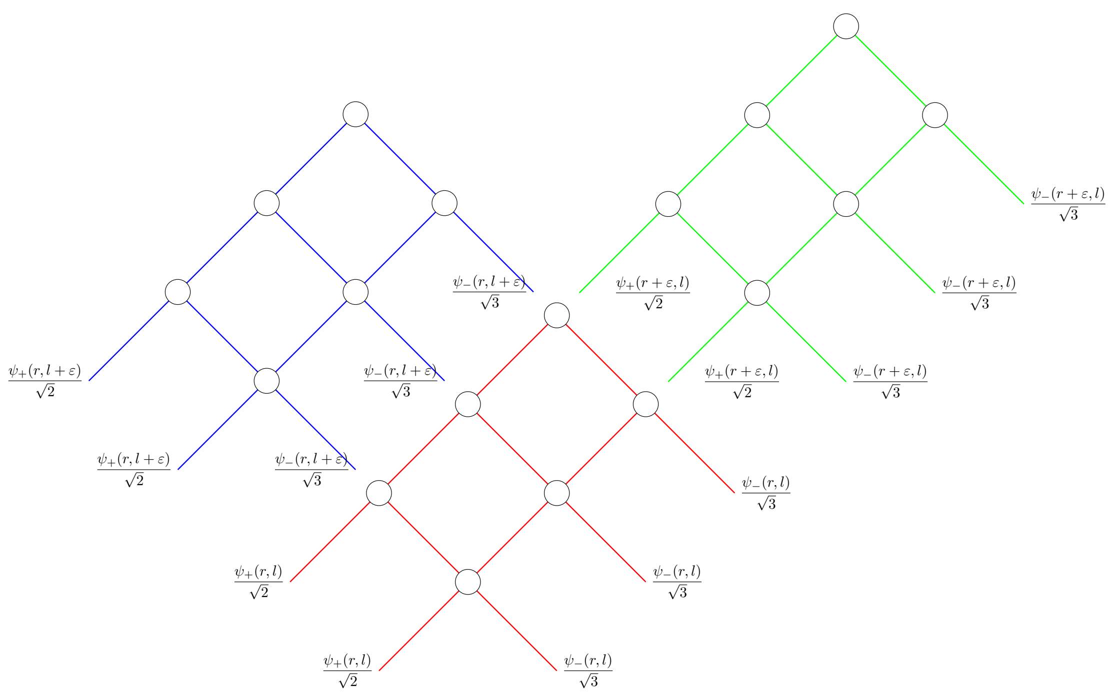
$$||\psi||_\sigma^2 = \int_\sigma j^s n_s d\sigma \tag{3.2.8}$$

where n_s is the unit normal vector to σ in r, l coordinates.

If ψ is a solution of the Dirac equation, then this definition does not actually depend on the surface σ (for a proof see for instance [Sch61b], Chap. 4), and so in this case we can write $||\psi||_\sigma^2 = ||\psi||^2$.



(a) Individual points and pairs incoming wires of the original spacetime diagram.



(b) Replacement by a rectangular patch of spacetime, which is a zoomed-in version of the point obtained by spreading out its incoming wires.

Figure 3.2.2: *A discrete Lorentz transform*, with parameters $\alpha = 3$, $\beta = 2$.

This definition of norm is Lorentz invariant, indeed:

$$\begin{aligned}
||\psi||^2_\sigma &= \int_\sigma j^s n_s d\sigma \\
&= \int_\sigma \left(\frac{|\psi_+|^2}{\beta} \beta dl + \frac{|\psi_-|^2}{\alpha} \alpha dr \right) \\
&= \int_{\sigma'} (|\psi'_+|^2 dl' + |\psi'_-|^2 dr') \\
&= \int_{\sigma'} j'^s n'_s d\sigma' \\
&= ||\psi'||^2_{\sigma'}
\end{aligned} \tag{3.2.9}$$

3.2.3.2 Discrete Cauchy surfaces

We now provide discrete counterparts to the above notions, beginning with *discrete Cauchy surfaces*. Let us consider a function $\sigma : \mathbb{Z} \to \{R, L\}$, and an origin (r_0, l_0). Together, they describe a piecewise linear curve made up of segments of the following form (in red): i.e.

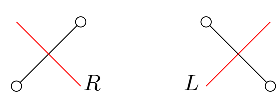


Figure 3.2.3: Breaking up of segments.

this curve intersects the spacetime lattice in two ways, labeled R and L (right, left). The centering on the origin is done as in Fig. 3.2.4 (a).

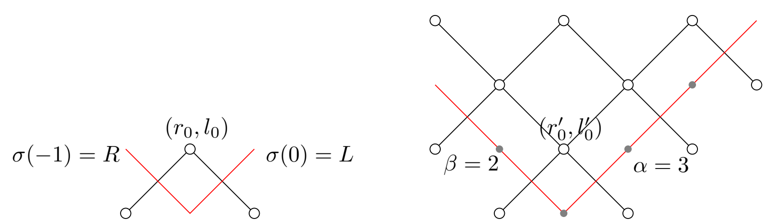


Figure 3.2.4: *Discrete Cauchy surfaces and their transformations.* (a) Centering on the origin (r_0, l_0) of the discrete Cauchy surface. (b) Lorentz transform of the same piece of surface for $\alpha = 3, \beta = 2$.

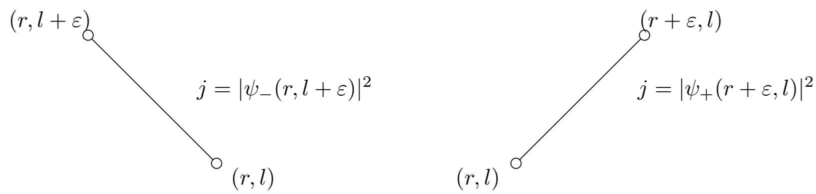
We say that such a curve is a *discrete Cauchy surface* if it does not contain infinite sequences of contiguous R or L. One can easily see that such a surface must intersect every lightlike curve exactly once. For concreteness, notice that the discrete equivalent to the continuous constant-time $t = 0$ Cauchy surface, is described by:

$$\sigma(n) = \begin{cases} L & \text{for even } n \\ R & \text{for odd } n \end{cases} \tag{3.2.10}$$

with origin $(0, 0)$.

3.2.3.3 Discrete current and discrete norm

Similarly, let us define the discrete current carried by a wavefunction ψ. At each wire connecting two points of the discrete lattice, the current is given by:



In analogy with the continuous case, we can evaluate the norm of ψ along a surface σ as follows

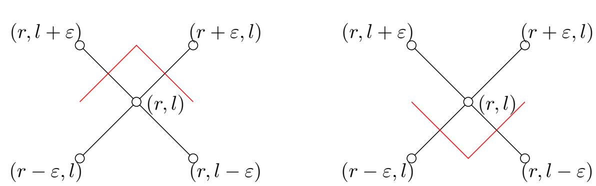
$$||\psi||^2_\sigma = \sum_{i \in \mathbb{Z}} j(i) \tag{3.2.11}$$

where $j(i)$ is the current of the wire at intersection i. For instance, for the discrete constant-time surface the above expression evaluates to the usual L_2-norm of a spacelike wavefunction

$$\begin{aligned} ||\psi||^2_{t=0} &= \sum_{i \in \mathbb{Z}} j(i) \\ &= \sum_{i \in 2\mathbb{Z}+1} |\psi_+(i, -i)|^2 + \sum_{i \in 2\mathbb{Z}} |\psi_-(i, -i)|^2 \\ &= \sum_i ||\psi(i, -i)||^2 = ||\psi||^2. \end{aligned} \tag{3.2.12}$$

3.2.3.4 Cauchy surface independence of the discrete norm

If ψ is a solution of a QW, then just like the continuous case, the discrete norm does not depend on the discrete Cauchy surface chosen for evaluating it. The proof outline is as follows. First, two Cauchy surfaces σ and σ' can be made to coincide on an arbitrary large region using only a finite sequence of swap moves[1]:



[1]We take the convention that if the swap move is applied to a segment around the origin, the origin moves along.

Second, swap moves leave the norm invariant, because of unitarity of the C gate (see Fig. 3.1.2):

$$|\psi_+(r+\varepsilon,l)|^2 + |\psi_-(r,l+\varepsilon)|^2 = |\psi_+(r,l)|^2 + |\psi_-(r,l)|^2. \tag{3.2.13}$$

Third, take a positive δ. By having σ to coincide with σ' on a large enough region, we obtain that $|(||\psi||_\sigma - ||\psi||_{\sigma'})| \leq \delta$. Lastly, since δ is arbitrary, $||\psi||_\sigma = ||\psi||_{\sigma'}$.

3.2.3.5 Lorentz invariance of the discrete norm

Finally, we will prove the analogue of equation (3.2.9) in the discrete setting. First of all we define how a discrete Cauchy surface σ transforms under a discrete Lorentz transform with parameters α, β. The sequence σ' is constructed from σ by replacing each L by L^α and each R with R^β, starting from the center. The origin (r_0, l_0) is mapped to the point $(r'_0, l'_0) = (\alpha r_0, \beta l_0)$. For instance, the piece of surface in Fig. 3.2.4(a) is transformed as in Fig. 3.2.4(b). We obtain (where $\mathcal{R}_\sigma$ and $\mathcal{L}_\sigma$ are the sets of right and left intersections respectively):

$$\begin{aligned}
||\psi||^2 &= \sum j(i) \\
&= \sum_{i\in\mathcal{R}_\sigma} |\psi_+(r_i,l_i)|^2 + \sum_{i\in\mathcal{L}_\sigma} |\psi_-(r_i,l_i)|^2 \\
&= \sum_{i\in\mathcal{R}_\sigma} \beta \left|\frac{\psi_+(r_i,l_i)}{\sqrt{\beta}}\right|^2 + \sum_{i\in\mathcal{L}_\sigma} \alpha \left|\frac{\psi_-(r_i,l_i)}{\sqrt{\alpha}}\right|^2 \\
&= \sum_{i'\in\mathcal{R}_{\sigma'}} |\psi'_+(r_{i'},l_{i'})|^2 + \sum_{i'\in\mathcal{L}_{\sigma'}} |\psi'_-(r_{i'},l_{i'})|^2 \\
&= \sum j'(i') = ||\psi'||^2.
\end{aligned} \tag{3.2.14}$$

3.2.4 The first-order-only Lorentz covariance of the Dirac QW

In Subsection 3.1.1 we defined the Dirac QW, and explained when a spacetime wavefunction ψ is a solution for it. In Subsection 3.2.2 we defined a discrete Lorentz transform, taking a spacetime wavefunction ψ into another spacetime wavefunction ψ'. In Subsection 3.2.3 we showed that this transformation preserves the norm, i.e. $||\psi||^2_\sigma = ||\psi'||^2_{\sigma'}$. The question that remains is whether the Dirac QW is Lorentz covariant with respect to this discrete Lorentz transform. In other words, is it the case that ψ' is itself a solution of the Dirac QW, for some m'? This demand is concrete translation of the main principle of special relativity, stating that the laws of physics (here, the Dirac QW) remain the same in all inertial reference frames (here, those of ψ and ψ').

Recall that the discrete Lorentz transform works by replacing each point of the spacetime lattice by a lightlike rectangular patch of spacetime, which can be understood as a "biased, zoomed in version" of that point, see Fig. 3.2.2. Internally, each patch is a piece of spacetime solution of the Dirac QW by construction, see Eq. (3.2.7). But is it the case that the patches match up, to form the entire spacetime wavefunction of a solution? After all, there could be inconsistencies in between patches: values carried by the incoming wires to the next patches, e.g. $\breve{\psi}_+(r+\varepsilon,l)$ (resp. $\breve{\psi}_-(r,l+\varepsilon)$) could be different from those carried by the wires coming out of the preceding patch, i.e. $\widehat{\psi}_+(r,l) = \overline{C}_+\breve{\psi}(r,l)$ (resp. $\widehat{\psi}_-(r,l) = \overline{C}_-\breve{\psi}(r,l)$). More precisely, we need both $\widehat{\psi}_+(r,l) = \breve{\psi}_+(r+\varepsilon,l)$ and $\widehat{\psi}_-(r,l) = \breve{\psi}_-(r,l+\varepsilon)$ for every r,l. This potential mismatch is represented by the discontinuations of the wires of Fig. 3.2.2(b). Clearly, the patches making up ψ' match up to form the spacetime wavefunction of a solution if and only if there are no such inconsistencies. We now evaluate these inconsistencies.

In the first order, the Dirac QW and the Finite-Difference Dirac equation are equivalent, as shown in Subsection 3.1.1. This makes it easier to compute the outcoming values of the patches, which should match the corresponding incoming wires (see Fig. A.1.1 in Appendix A.1). Let $m' = m/\sqrt{\alpha\beta}$. In general, we obtain (to first order in ε, for $i = 0\dots\beta-1$, $j = 0\dots\alpha-1$):

$$\begin{aligned}
\widehat{\psi}_+(r,l)_i &= \left(\overline{C}_+\breve{\psi}(r,l)\right)_i \\
&= \frac{\psi_+(r,l)}{\sqrt{\beta}} - \alpha \mathrm{i} m'\varepsilon\frac{\psi_-(r,l)}{\sqrt{\alpha}} \\
&= \frac{\psi_+(r,l) - \mathrm{i}m\varepsilon\psi_-(r,l)}{\sqrt{\beta}} \\
&= \breve{\psi}_+(r+\varepsilon,l)_i \\
\text{and} \qquad \widehat{\psi}_-(r,l)_j &= \left(\overline{C}_-\breve{\psi}(r,l)\right)_j \\
&= \frac{\psi_-(r,l)}{\sqrt{\alpha}} - \beta \mathrm{i} m'\varepsilon\frac{\psi_+(r,l)}{\sqrt{\beta}} \\
&= \frac{\psi_-(r,l) - \mathrm{i}m\varepsilon\psi_+(r,l)}{\sqrt{\alpha}} \\
&= \breve{\psi}_-(r,l+\varepsilon)_j.
\end{aligned}$$

Hence, the wires do match up in the first order. However, the second order cannot be fixed, even if we allow for arbitrary encodings. The detailed proof of this statement is left to Appendix A.

The lack of second order covariance of the Dirac QW can be interpreted in several ways. First, as saying that the Dirac QW is not a realistic model. This interpretation motivates us to explore, in the next sections, the question whether other discrete models (QWs or QCA) could not suffer this downside, and be exactly covariant. Second, as an indication that Lorentz covariance breaks down at Planck scale. Third, as saying that we have no choice but to view ε as an infinitesimal, so that we can ignore its second order. In this picture, the Dirac QW would be understood as describing an infinitesimal time evolution, but in the same formalism as that of discrete time evolutions, i.e. in an alternative language to the Hamiltonian formalism. Formulating an infinitesimal time quantum evolution in such a way has an advantage: it sticks to the language of unitary, causal operators [ANW11a] and readily provides a quantum simulation algorithm.

3.2.5 Transformation of velocities

In Subsection 3.2.2 we defined a discrete Lorentz transform, which takes a spacetime wavefunction ψ into a Lorentz transformed wavefunction ψ'. In Subsection 3.2.4 we proved that the Dirac QW is first-order covariant. Is it the case that the velocity of ψ is related to the velocity of ψ' according to the transformation of velocity rule of special relativity? We will show that it is indeed the case, so long as we transform the "local velocity field" $v(r,l)$, defined as:

$$v(r,l) = \frac{|\psi_+(r,l)|^2 - |\psi_-(r,l)|^2}{||\psi(r,l)||^2}. \tag{3.2.15}$$

In order to see how we arrive at this formula, let us first recall the definition of velocity in the continuous case.

For the Dirac equation, the velocity operator is obtained via the Heisenberg formula, $d\hat{x}/dt = \mathrm{i}[H,\hat{x}] = \sigma_3$ (see Eq. (3.1.1)). Thus, in the discrete setting it is natural to define the velocity operator as $\Delta X = X - WXW^\dagger$, where X is the position operator, $X = \sum_x xP_x = \sum_x x|x\rangle\langle x|$ and $W = TC$ is the walk operator. We have

$$\begin{aligned}\Delta X &= X - WXW^\dagger = X - TCXC^\dagger T^\dagger = X - TXT^\dagger \\ &= \begin{pmatrix} \sum_x xP_x & 0 \\ 0 & \sum_x xP_x \end{pmatrix} - \begin{pmatrix} \sum_x xP_{x+1} & 0 \\ 0 & \sum_x xP_{x-1} \end{pmatrix} \\ &= \sigma_3 \end{aligned} \tag{3.2.16}$$

Thus the expected value of ΔX at the time slice $t=0$ is, as in the continuous case,

$$\begin{aligned}\langle\sigma_3\rangle_\psi &= \sum_{i\in\mathbb{Z}} |\psi_+(i,-i)|^2 - |\psi_-(i,-i)|^2 \\ &= \sum_{i\in\mathbb{Z}} p(i,-i)v(i,-i) \end{aligned} \tag{3.2.17}$$

where $p(r,l) = ||\psi(r,l)||^2$. It should be noted that it is not a constant of motion. This is in fact a manifestation of the Zitterbewegung, whose connection with the continuous case was well studied by several authors [Str07, BDT13, Kur08]. Eq. (3.2.17) justifies our definition of local velocity.

Let us now consider the case of a walker which at $t=0$, $x=0$, has internal degree of freedom $\psi = (\psi_+,\psi_-)^\mathsf{T}$. We will relate $v = v(0,0)$ and $v' = v'(0,0)$ as calculated from a Lorentz transformed observer with parameters α,β. We have $v = (|\psi_+|^2 - |\psi_-|^2)/||\psi||^2$. We can deduce $|\psi_+|^2 = ||\psi||^2(1+v)/2$ and $|\psi_-|^2 = ||\psi||^2(1-v)/2$. Now, let us apply a discrete Lorentz transform. At point $(0,0)$, it takes ψ into $\psi' = S\psi$, whose corresponding velocity is:

$$\begin{aligned} v' &= \frac{|\psi'_+|^2 - |\psi'_-|^2}{||\psi'||^2} = \frac{\alpha|\psi_+|^2 - \beta|\psi_-|^2}{\alpha|\psi_+|^2 + \beta|\psi_-|^2} \\ &= \frac{\alpha||\psi||^2(1+v) - \beta||\psi||^2(1-v)}{\alpha||\psi||^2(1+v) + \beta||\psi||^2(1-v)} \\ &= \frac{v + \frac{\alpha-\beta}{\alpha+\beta}}{1 + v\frac{\alpha-\beta}{\alpha+\beta}} \\ &= \frac{v+u}{1+vu} \end{aligned} \tag{3.2.18}$$

where $u = (\alpha-\beta)/(\alpha+\beta)$ is the velocity that corresponds to the discrete Lorentz transform with parameters α, β. Thus the local velocity associated to a spacetime wavefunction ψ is related to the local velocity of the corresponding Lorentz transformed ψ' by the rule of addition of velocities of special relativity.

3.3 Formalization of Discrete Lorentz covariance in general

We will now provide a formal, general notion of discrete Lorentz transform and Lorentz covariance for Quantum Walks and Quantum Cellular Automata.

3.3.1 Over Quantum Walks

Beforehand, we need to explain which general form we assume for Quantum Walks.

3.3.1.1 General form of Quantum Walks

Intuitively speaking, a Quantum Walk (QW) is a single particle or walker moving in discrete-time steps on a lattice. Axiomatically speaking, QWs are shift-invariant, causal, unitary evolutions over the space $\bigoplus_{\mathbb{Z}} \mathcal{H}_c$, where c is the dimension of the internal degrees of freedom of the walker. Constructively speaking, in turns out [GNVW12, SW04, ANW08] that, at the cost of some simple recodings, any QW can be put in a form which is similar to that of the circuit for the Dirac QW shown Fig. 3.1.2(c). In general, however, c may be larger than 2 (the case c equal 1 is trivial [Mey96]). But it can always be taken to be even, so that the general shape for the circuit of a QW can be expressed as in Fig. 3.3.1. Notice how, in this diagram, each wire carries a d-dimensional vector $\psi_\pm(r,l)$. We will say that the QW has 'wire dimension' d. Incoming wires get composed together with a direct sum, to form a $2d$-dimensional vector $\psi(r,l)$. The state $\psi(r,l)$ undergoes a $2d \times 2d$ unitary gate C to become some $\psi'(r,l) = \psi'_+(r+\varepsilon,l) \oplus \psi'_-(r,l+\varepsilon)$, etc. The unitary gate C is called the 'coin'. Algebraically speaking, this means that a QW can always be assumed to be of the form:

$$\mathrm{diag} e^{\varepsilon\partial_r}\, \mathrm{Id}_d e^{\varepsilon\partial_l}\, \mathrm{Id}_d \psi = C\psi. \tag{3.3.1}$$

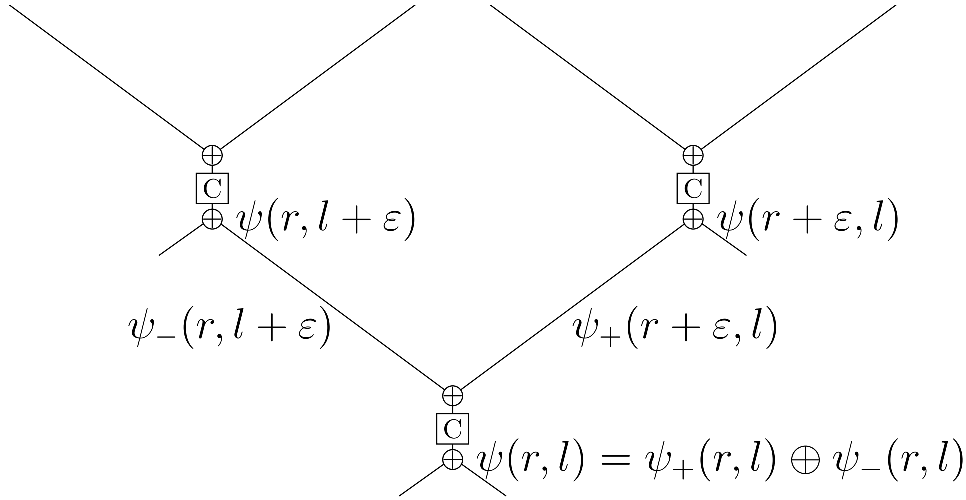


Figure 3.3.1: *The circuit for a general QW.* The wire dimension is d, meaning that $\psi_+(r,l) = (\psi_+^1(r,l), \ldots, \psi_+^d(r,l))^\mathsf{T}$, etc.

We will not, in this chapter, consider QW with additional wires (i.e. more complicated neighbourhoods) as the resulting theory would be convoluted, and because they do not fit well with the picture of a lightspeed $c = 1$. Again, they can always be brought back into the above form via space grouping of adjacent cells into supercells [ANW08, ANW11b].

3.3.1.2 Lorentz transforms for QW

The formalization of a general notion of Lorentz transform for QWs generalizes that presented in Section 3.2. Consider a QW having wire dimension d, and whose $2d \times 2d$ unitary coin is C_m, where the m are parameters (In the case of the Dirac QW the coin is given explicitly in 3.1.1 and there the only parameter is the mass. However, keep in mind that in general m stands for any set of parameters.). A Lorentz transform $L_{\alpha,\beta}$ is specified by:

- a function $m' = f_{\alpha,\beta}(m)$, such that $f_{\alpha'\alpha,\beta'\beta} = f_{\alpha',\beta'} \circ f_{\alpha,\beta}$.
- a family of isometries E_α from $\mathcal{H}_d$ to $\bigoplus_\alpha \mathcal{H}_d$, such that $(\bigoplus_\alpha E_{\alpha'})E_\alpha = E_{\alpha'\alpha}$.

Above we used the notation $\bigoplus_\alpha \mathcal{H}_d = \bigoplus_{i=1\ldots\alpha} \mathcal{H}_d$. Consider ψ a spacetime wavefunction (at this stage it is not necessary to assume that it is a solution of the QW). Switching to lightlike coordinates, its Lorentz transform $\psi' = L_{\alpha,\beta}\psi$ is obtained by:

- for every (r,l), computing: $\breve{\psi}_+ = E_\beta \psi_+$, $\breve{\psi}_- = E_\alpha \psi_-$, and $\breve{\psi} = \breve{\psi}_+ \oplus \breve{\psi}_- = \overline{E}\psi$.
- for every (r,l), replacing: the point (r,l) by the lightlike $\alpha \times \beta$ rectangular patch of spacetime

$$\left(\overline{C}_{m'}(i,j)\breve{\psi}(r,l)\right)_{i=0\ldots\alpha-1, j=0\ldots\beta-1} \tag{3.3.2}$$

with $\overline{C}_{m'}(i,j)$ as in Remark 3.1 and Fig. 3.1.3.

Again, Fig. 3.2.2 illustrated an example of such a transformation, for the case of the Dirac QW. The corresponding isometries E_α, described in section 3.2.2, are given by

$$E_\alpha = \frac{1}{\sqrt{\alpha}}\mathbf{1}_\alpha \tag{3.3.3}$$

where $\mathbf{1}_d = (1,\dots,1)^\mathsf{T}$ is the d-dimensional uniform vector, and the function $f_{\alpha,\beta}$ is given by $f_{\alpha,\beta}(m) = m/\sqrt{\alpha\beta}$.

Notice that while the focus of this chapter is on translation-invariant QW, this is not actually required in order to define the Lorentz transform. The same definition would apply equally well if the QW has parameters that depend on the position, i.e. $m = m(r,l)$. We just note that in this case, according to our definition, $f_{\alpha,\beta}$ will not itself depend on the position, and that the new parameters m' would be constant over each lightlike rectangular patch.

3.3.1.3 Lorentz covariance for QW

The formalization of a general notion of Lorentz covariance for QWs generalizes that presented in Subsection 3.2.4. Consider a QW having wire dimension d whose $2d \times 2d$ and unitary coin unitary coin C_m, where the m are parameters. Consider ψ a spacetime wavefunction which is a solution of this QW. We just gave the formalization of a discrete general notion of Lorentz transform taking a spacetime wavefunction ψ into another spacetime wavefunction $\psi' = L_{\alpha,\beta}\psi$, and parameters m into m'. Is it the case, for any α and β, that the spacetime wavefunction ψ' is a solution of the same QW, but with parameters m'? If so, the QW is said to be covariant with respect to the given discrete Lorentz transform. Now, the above-defined discrete Lorentz transform is obtained by replacing each point with a lightlike $\alpha \times \beta$ rectangular patch of spacetime, which, by definition, is internally a piece of spacetime solution of the Dirac QW see Eq. (3.3.2). But again, is it the case that the patches match up to form the entire spacetime wavefunction of a solution? Let us again define

$$\widehat{\psi}_+(r,l) = (\overline{C}_{m'})_+\widecheck{\psi}(r,l) \quad \text{and} \quad \widehat{\psi}_-(r,l) = (\overline{C}_{m'})_-\widecheck{\psi}(r,l). \tag{3.3.4}$$

We need: $\widehat{\psi}_+(r,l) = \widecheck{\psi}_+(r+\varepsilon,l)$ and $\widehat{\psi}_-(r,l) = \widecheck{\psi}_-(r,l+\varepsilon)$. An equivalent, algebraic way of stating these two requirements is obtained as follows:

$$\widecheck{\psi}_+(r+\varepsilon,l) \oplus \widecheck{\psi}_-(r,l+\varepsilon) = \widehat{\psi}_+(r,l) \oplus \widehat{\psi}_-(r,l)$$

Equivalently,

$$\begin{aligned}
&(E_\beta \oplus E_\alpha)\left(\psi_+(r+\varepsilon, l) \oplus \psi_-(r, l+\varepsilon)\right) = \\
&\left(\overline{C}_{m'}(\alpha, \cdot) \oplus \overline{C}_{m'}(\cdot, \beta)\right)(E_\beta \oplus E_\alpha)\,\psi(r,l) \\
\Leftrightarrow &(E_\beta \oplus E_\alpha)\, C_m \psi(r,l) = \overline{C}_{m'}\,(E_\beta \oplus E_\alpha)\,\psi(r,l) \\
\Leftrightarrow &(E_\beta \oplus E_\alpha)\, C_m = \overline{C}_{m'}\,(E_\beta \oplus E_\alpha) \\
\Leftrightarrow &\overline{E} C_m = \overline{C}_{m'} \overline{E}.
\end{aligned} \tag{3.3.5}$$

Notice that in the non-translation invariant case where $m = m(r, l)$, the above is required for every possible values that m can take.
This expresses discrete Lorentz covariance elegantly, as a form of commutation relation between the evolution and the encoding. Diagrammatically this is represented by Fig. 3.3.2(a). The isometry of the E_α can also be represented diagrammatically, cf. Fig. 3.3.2(b). Combining both properties straightforwardly leads to

$$C_m = \overline{E}^\dagger \overline{C}_{m'} \overline{E}. \tag{3.3.6}$$

This is represented as Fig. 3.3.3(a), which of course can be derived diagrammatically from Fig. 3.3.2. Is this diagrammatic theory powerful enough to be considered an abstract, pictorial theory of Lorentz covariance, in the spirit of [Coe10]?

3.3.1.4 Diagrammatic Lorentz covariance for QW

Combining the diagrammatic equalities of Fig. 3.3.2, we can almost rewrite the spacetime circuit of a QW with coin C_m, into its Lorentz transformed version, for any parameters $\alpha, \beta \ldots$ but not quite. A closer inspection shows that this can only be done over regions such as past cones, by successively: 1/ Introducing pairs of encodings via rule Fig. 3.3.2(b) along the border of the past cone; 2/ Pushing back towards the past the bottom E via rule Fig. 3.3.2(a), thereby unveiling the Lorentz transformed past cone. Whilst this limitation to past-cone-like regions may seem surprising at first, there is a good intuitive reason for that. Indeed, the diagrammatic equalities of Fig. 3.3.2 tell you that you can locally zoom into a spacetime circuit; but you can only locally zoom out if you had zoomed in earlier, otherwise there may be a loss of information. This asymmetry is captured by the fact that Fig. 3.3.2(a) cannot be put upside-down, time-reversed. It follows that you should not be able to equalize an entire spacetime circuit with its complete Lorentz transform, at least not without using further hypotheses. And indeed, when we local Lorentz transform an entire past cone, its border is there to keep track of the fact that this region was locally zoomed into, and that we may later unzoom from it, if we want.

Now, could we add a further diagrammatic rule which would allow us to perform an complete Lorentz transformation, perhaps at the cost of annotating our spacetime circuit diagrams with information on whom has been zoomed into? Those annotations are the dashed lines of Fig. 3.3.2 and Fig. 3.3.3(a). Clearly, as we use those rules, we know whether some bunch of wires lives in the subspace S_α of the projector $E_\alpha E_\alpha^\dagger$, and we can

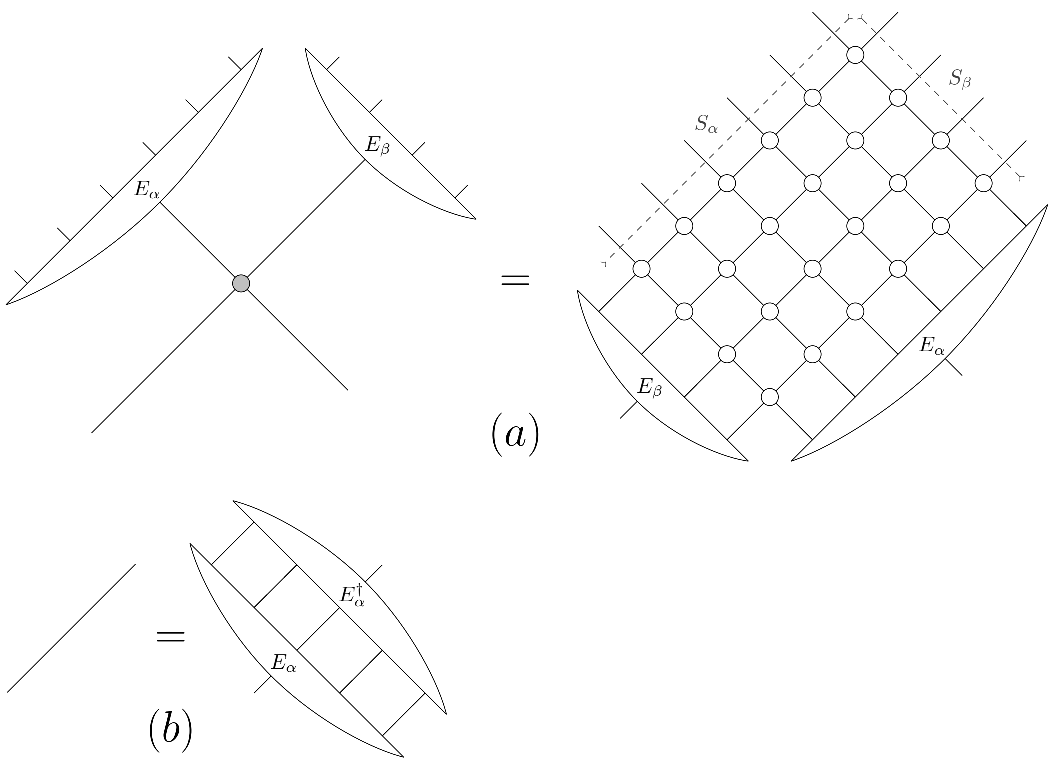


Figure 3.3.2: *Basic covariance rules*. (a) Expresses the fundamental covariance condition of Eqs. (3.3.5) and (3.3.11). The dashed line is optional, it is an indication which results from using this rule: it tells us that the state of these wires belongs to the subspace S_α. The gray and white dots stand for the same unitary interaction, but with different parameters. (b) Expresses the isometry of the encodings used for the discrete Lorentz transform.

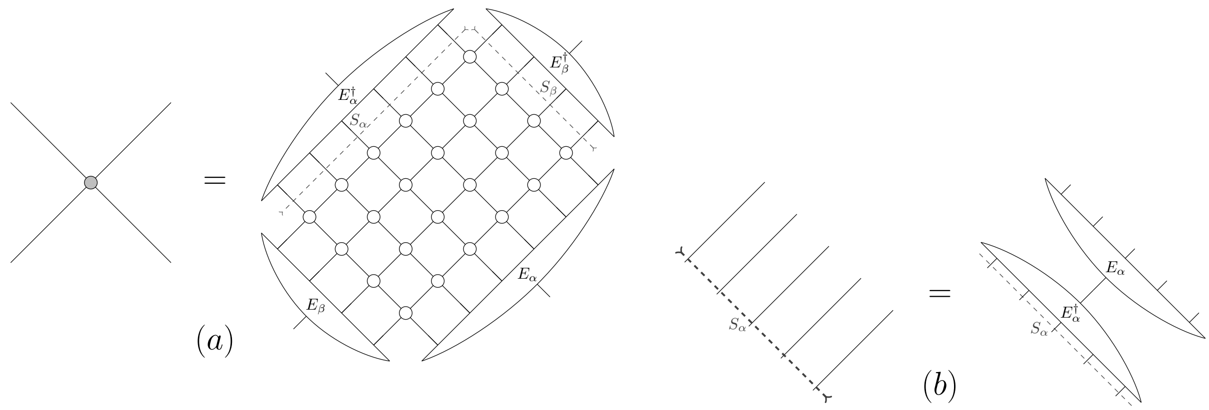


Figure 3.3.3: *Completed covariance rules*. (a) is a theorem, derived from the diagrams of Fig. 3.3.2, see also Eqs (3.3.6) and (3.3.12). It expresses the idea of a Lorentz transform being a zoom in. The dashed line is optional, it is an indication which results from using this rule: it tells us that the state of these wires belongs to the subspace S_α. The gray and white dots stand for same unitary interaction, but with different parameters. (b) is a conditional rule: the thicker dashed line is a precondition for the equality to hold. Again it follows from the isometry of the encodings used for the discrete Lorentz transform, see also Eq. (3.3.7).

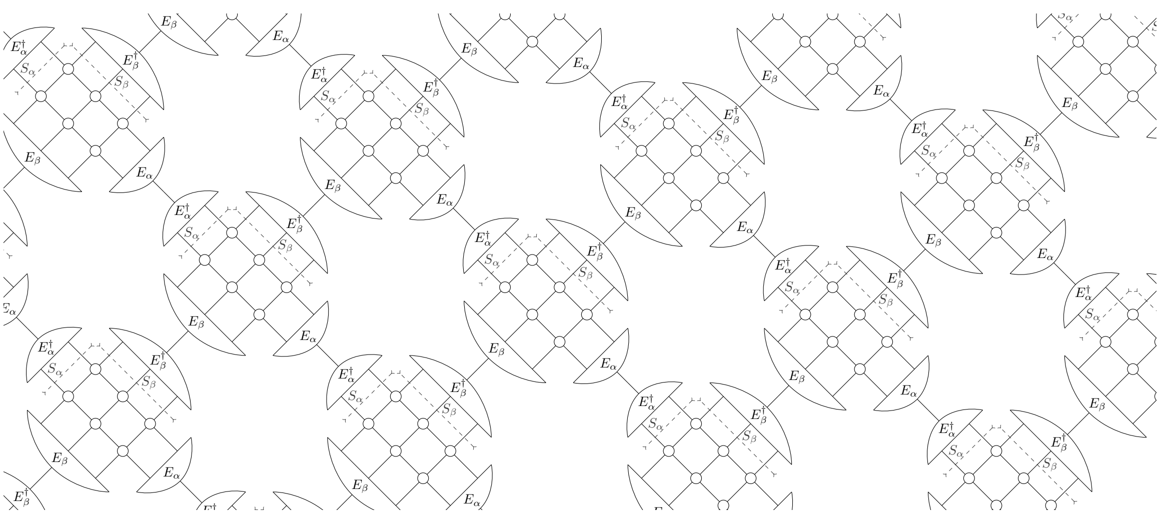


Figure 3.3.4: *Performing a complete Lorentz transform via the completed covariance rules*. A Lorentz transform with parameters $\alpha = 2$ and $\beta = 3$ consists in replacing each point by a 2×3 rectangular patch of spacetime using isometric encodings.

leave that information behind. Moreover, on this subspace, it is the case that

$$E_\alpha E_\alpha^\dagger = \mathrm{Id}_{S_\alpha}\,. \tag{3.3.7}$$

Then, representing this last equation in rule Fig. 3.3.3(b), which is conditional on the annotation being there (the other rules are non-conditional, they provide the annotations), we reach our purpose. Indeed, in order to perform a complete Lorentz-transform we can now apply the rule Fig. 3.3.3(a) everywhere, leading to Fig. 3.3.4, and then remove the encoding gates everywhere via Fig. 3.3.3(b). Thus, it could be said that the rewrite rules of Fig. 3.3.3 provide an abstract, pictorial theory of Lorentz covariance. They allow to equalize, spacetime seen by a certain observer, with spacetime seen by another, inertial observer. Besides their simplicity, the local nature of the rewrite rules is evocative of the local Lorentz covariance of General Relativity. This is explored a little further in Subsection 3.3.3.

3.3.1.5 Inverse transformations and equivalence upon rescaling

In analogy with the continuum case, we would like the inverse of a Lorentz transform $L_{\alpha,\beta}$ to be $L_{\beta,\alpha}$, i.e.

$$L_{\alpha,\beta}L_{\beta,\alpha} = \mathrm{Id}\,. \tag{3.3.8}$$

However, according our definitions of $L_{.,.}$, we know that $L_{\alpha,\beta}L_{\beta,\alpha}$ is a transformation such that

- each point (r,l) is replaced by the lightlike $\alpha\beta\times\alpha\beta$ square patch of spacetime, with left-incoming wires $F\psi_+(r,l)$, right-incoming wires $F\psi_-(r,l)$, right-outgoing wires $F\psi_+(r+\varepsilon,l)$ and left-outgoing wires $F\psi_-(r,l+\varepsilon)$, where

$$F = \left(\bigoplus_\alpha E_\beta\right) E_\alpha = E_{\beta\alpha} = E_{\alpha\beta} = \left(\bigoplus_\beta E_\alpha\right) E_\beta \tag{3.3.9}$$

- the coin parameter m is mapped to $m' = f_{\alpha\beta,\alpha\beta}(m)$.

Hence, if we are to claim (3.3.8) we need to identify any two spacetime diagrams which satisfy these relations. This is achieved as a special case in the completed diagrammatic theory of Fig. 3.3.3.

3.3.2 Over Quantum Cellular Automata

3.3.2.1 General form of Quantum Cellular Automata

Intuitively speaking, a Quantum Cellular Automata (QCA) is a multiple walkers QW. The walkers may or may not interact, their numbers may or may not be conserved. Axiomatically speaking, a QCA is a shift-invariant, causal, unitary evolution over the space "$\bigotimes_{\mathbb{Z}}\mathcal{H}_c$", where c is the dimension of the internal degrees of freedom of each site. Actually, care must be taken when defining such infinite tensor products, but two solutions

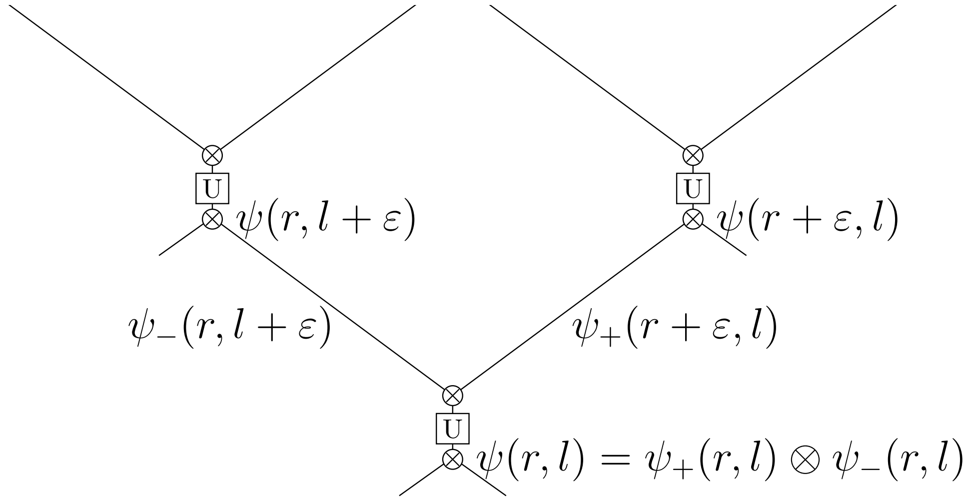


Figure 3.3.5: *The circuit for a general QCA.*

exist [SW04, ANW08, ANW11b]. Constructively speaking, it turns out [SW04, ANW08, ANW11b] that, at the cost of some simple recodings, any QCA can be put in the form of a quantum circuit. This circuit can then be simplified [AG12] to bear strong resemblance with the circuit of a general QW seen in Fig. 3.3.1. In particular c can always be taken to be d^2, so that the general shape for the quantum circuit of a QCA is that of Fig. 3.3.5. Notice how, in this diagram, each wire carries a d-dimensional vector $\psi_\pm(r,l)$. We will say that the QCA has 'wire dimension' d. Incoming wires get composed together with a tensor product, to form a d^2-dimensional vector $\psi(r,l)$. The state $\psi(r,l)$ undergoes a $d^2 \times d^2$ unitary gate U to become some $\psi_+(r+\varepsilon,l) \otimes \psi_-(r,l+\varepsilon)$, etc. The unitary gate U is called the 'scattering operator'. Notice how, to some extent, the QCA are alike QW up to replacing $\oplus$ by $\otimes$. Algebraically speaking, the above means that one time-step of a QCA can always be assumed to be of the form:

$$\psi \mapsto \left(\bigotimes_{2\mathbb{Z}+1} U \right) \left(\bigotimes_{2\mathbb{Z}} U \right) \psi. \tag{3.3.10}$$

3.3.2.2 Lorentz transforms for QCA

The formalization of a general notion of Lorentz transform for QCA is obtained from that over QW essentially by changing occurrences of $\oplus$ into $\otimes$. Indeed, consider a QCA having wire dimension d, and whose $d^2 \times d^2$ unitary scattering operator U has parameters m. A Lorentz transform $L_{\alpha,\beta}$ is specified by:

- a function $m' = f_{\alpha,\beta}(m)$ such that $f_{\alpha'\alpha,\beta'\beta} = f_{\alpha',\beta'} \circ f_{\alpha,\beta}$.
- a family of isometries E_α from $\mathcal{H}_d$ to $\bigotimes_\alpha \mathcal{H}_d$, such that $(\bigotimes_\alpha E_{\alpha'})E_\alpha = E_{\alpha'\alpha}$.

There is a crucial difference with QWs, however, which is that we cannot easily apply this discrete Lorentz transform to a spacetime wavefunction. Indeed, consider ψ a spacetime wavefunction. For every time t, the state $\psi(t)$ may be a large entangled state across space. What meaning does it have, then, to select another spacelike surface? What meaning does it have to switch to lightlike coordinates? Unfortunately the techniques which were our point of departure for QWs, no longer apply. Fortunately, the algebraic and diagrammatic techniques which were our point of arrival for QWs, apply equally well to QCA, so that we may still speak of Lorentz-covariance.

3.3.2.3 Lorentz covariance for QCA

Again, the formalization of the notion of Lorentz-covariance for QCA cannot be given in terms of ψ' being a solution if ψ was a solution, because we struggle to speak of ψ'. Instead, we define Lorentz-covariance straight from the algebraic view:

$$\begin{aligned}(E_\beta \otimes E_\alpha)\, U_m &= \overline{U}_{m'}\, (E_\beta \otimes E_\alpha) \\ \text{i.e.} \quad \overline{E} U_m &= \overline{U}_{m'} \overline{E}.\end{aligned} \tag{3.3.11}$$

Diagrammatically this is represented by the same figure as for QWs, namely Fig. 3.3.2(a). The isometry of the E_α is again represented by Fig. 3.3.2(b). Algebraically speaking, combining both properties again leads to

$$U_m = \overline{E}^\dagger \overline{U}_{m'} \overline{E}. \tag{3.3.12}$$

Which diagrammatically this is again represented as Fig. 3.3.3(a). For the same reasons, the conditional rule Fig. 3.3.3(b) again applies: the whole diagrammatic theory carries through unchanged from QWs to QCA.

3.3.3 Non-homogeneous discrete Lorentz transforms and non-inertial observers

Nothing in the above developed diagrammatic theory forbids us to apply different local discrete Lorentz transforms to different points of spacetime, so long as point (r, l) and point $(r + \varepsilon, l)$ (resp. point $(r, l + \varepsilon)$) have the same parameter β (resp. α). This constraint propagates along lightlike lines, so that there can be, at most, one different α_r (resp. β_l) per right-moving (resp. left-moving) lightlike line r (resp. l). We call this a non-homogeneous discrete Lorentz transform of parameters (α_r), (β_l).

The circuit which results from applying such a non-homogeneous discrete Lorentz transform is, in general, a non-homogeneous QWs (resp. QCA), as it may lack shift-invariance in time and space. This is because the coin C_m (resp. scattering unitary U_m) of the point (r, l) gets mapped into lightlike $\alpha_r\beta_l$-rectangular patch of spacetime $\overline{C}_{m'}$ (resp. $\overline{U}_{m'}$), whose parameters $m' = f_{\alpha_r,\beta_l}(m)$ may depend, in general, upon the position (r, l). This problem is avoided if $f_{\alpha\beta} = f$ does not depend upon α and β, as in the example which will be introduced in Section 3.5.

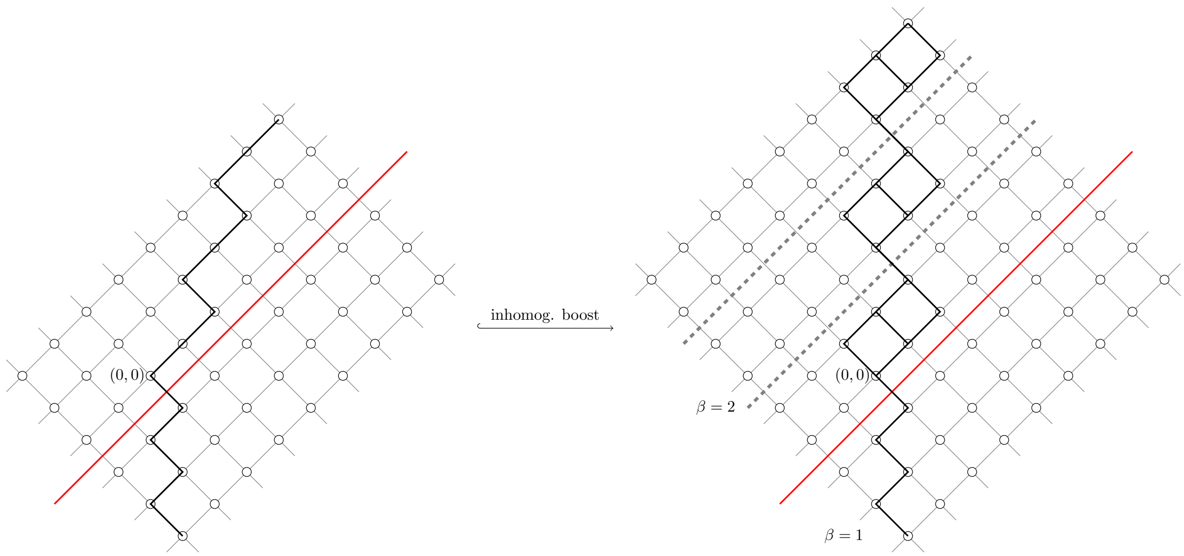


Figure 3.3.6: *An inhomogeneous transformation for a non-inertial observer.* The region above the red line undergoes a Lorentz transform with parameters $\alpha = 1$ and $\beta = 2$, whilst the region below is left unchanged. After the inhomogeneous transformation, the observer is at rest.

Provided that the condition $f_{\alpha\beta} = f$ is met, we can now transform between non-inertial observers by a non-homogeneous discrete Lorentz transform. Figure 3.3.6 illustrates this with the simple example of an observer which moves one step right, one step left, until it reaches point $(0, 0)$ where it gets accelerated, and continues moving two steps right, one step left etc. We choose $\beta_l = 1$ for $l < 0$,$\beta_l = 2$ for $l \geq 0$ and $\alpha_r = 1$ for all r. This has the effect of slowing down the observer just beyond the point $(0, 0)$. All along his trajectory, he now has to move two steps right for every two steps left that he takes, so that he is now at rest.

In general, suppose that an observer moves a_k steps to the right, b_k steps left, a_{k+1} steps right, etc. He does this starting from position $r_k = r_{k-1} + a_k$ and $l_k = l_{k-1} + b_k$. For every k, let M_k be the least common multiple of a_k and b_k. We choose $\alpha_r = M_k/a_k$ for $r_{k-1} \leq r < r_k$ and $\beta_l = M_k/b_k$ for $l_{k-1} \leq l < l_k$. Let us perform the non-homogeneous discrete Lorentz transform of parameters (α_r), (β_l). Then, the observer now moves M_k steps right for every M_k steps left he takes, and then M_{k+1} steps right for every M_{k+1} steps left, etc.

3.4 The Clock QW

Equipped with a formal, general notion of Lorentz transform and Lorentz covariance for QW, we can now seek for an exactly covariant QW.

3.4.1 Definition

In the classical setting, covariance of random walks has already been explored [Wal88]. The random walk of [Wal88] uses a fair coin, but is nonetheless biased in the following way: after a (fair) coin toss the walker moves during p time steps to the right (resp. during q time steps to the left). There is a reference frame in which the probability distribution is symmetric, namely that with velocity $u = (p-q)/(p+q)$. Changing the parameters p and q corresponds to performing a Lorentz transform of the spacetime diagram.

Now we will make an analogous construction in the quantum setting. The main point is to enlarge the coin space so that the coin operator is idle during p, or q, time steps. The coin space will be $\mathcal{H}_C = \mathcal{H}_C^+ \oplus \mathcal{H}_C^-$, where $\mathcal{H}_C^+ \cong \mathcal{H}_C^- = \ell^2(\mathbb{Q}^{\geq 0})$. The Hilbert space of the quantum walk is then $\mathcal{H} = \ell^2(\mathbb{Z}) \otimes \mathcal{H}_C$, whose basis states will be indicated by $|x, h^s\rangle$, with $h \in \mathbb{Q}^{\geq 0}$, $s = \pm$.

This $\mathcal{H}_C^\pm$ will act as a "counter". When $h > 0$, the walker moves without interaction and the counter is decreased. When the counter reaches 0, the effective coin operator is applied and the counter is reset.

The evolution of the Clock QW with parameters p, q is defined on the subspace $\mathcal{H}_C^{p,q}$ of $\mathcal{H}_C$ spanned by the $p+q$ vectors $\{|\frac{i}{p}^+\rangle, |\frac{j}{q}^-\rangle\}$ with $i = 0, \ldots, p-1$ and $j = 0, \ldots, q-1$, as follows:

$$W_{p,q}|x, h^s\rangle = \begin{cases} |x+1, (h-\frac{1}{p})^+\rangle & \text{for } s=+, \quad 0 < h \leq 1-\frac{1}{p} \\ |x-1, (h-\frac{1}{q})^-\rangle & \text{for } s=-, \quad 0 < h \leq 1-\frac{1}{q} \\ a|x+1, (1-\frac{1}{p})^+\rangle + b|x-1, (1-\frac{1}{q})^-\rangle & \text{for } s=+, \quad h=0 \\ c|x+1, (1-\frac{1}{p})^+\rangle + d|x-1, (1-\frac{1}{q})^-\rangle & \text{for } s=-, \quad h=0 \end{cases} \tag{3.4.1}$$

This map is unitary provided that the 2×2 matrix C of coefficients $C_{11} = a$, $C_{12} = b$, $C_{21} = c$, $C_{22} = d$ is unitary. For instance we could choose, as for the Dirac QW, $a = d = \cos(m\varepsilon)$, $b = c = -\mathrm{i}\sin(m\varepsilon)$.

The Clock QW with parameters p and q will only be used over $\ell^2(\mathbb{Z}) \otimes \mathcal{H}_C^{p,q}$ where it admits a matrix form which we now provide (over the rest of $\mathcal{H}_C$ it can be assumed to be the identity). From Eq. (3.4.1) we can write $W_{p,q} = T_{p,q}C_{p,q}$ where $T_{p,q}$ is the shift operator,

$$T_{p,q} = \text{diag}\left(\overbrace{e^{-\varepsilon\partial_x}, \ldots, e^{-\varepsilon\partial_x}}^{p \text{ times}}, \overbrace{e^{\varepsilon\partial_x}, \ldots, e^{\varepsilon\partial_x}}^{q \text{ times}}\right) \tag{3.4.2}$$

and $C_{p,q}$ is the coin operator:

$$C_{p,q} = \left(\begin{array}{cc|cc} 0 & \mathrm{Id}_{p-1} & 0 & 0 \\ a & 0 & b & 0 \\ \hline 0 & 0 & 0 & \mathrm{Id}_{q-1} \\ c & 0 & d & 0 \end{array}\right). \tag{3.4.3}$$

Hence, the Clock QW has an effective coin space of finite dimension $p+q$. However, we will see that this dimension changes under Lorentz transforms.

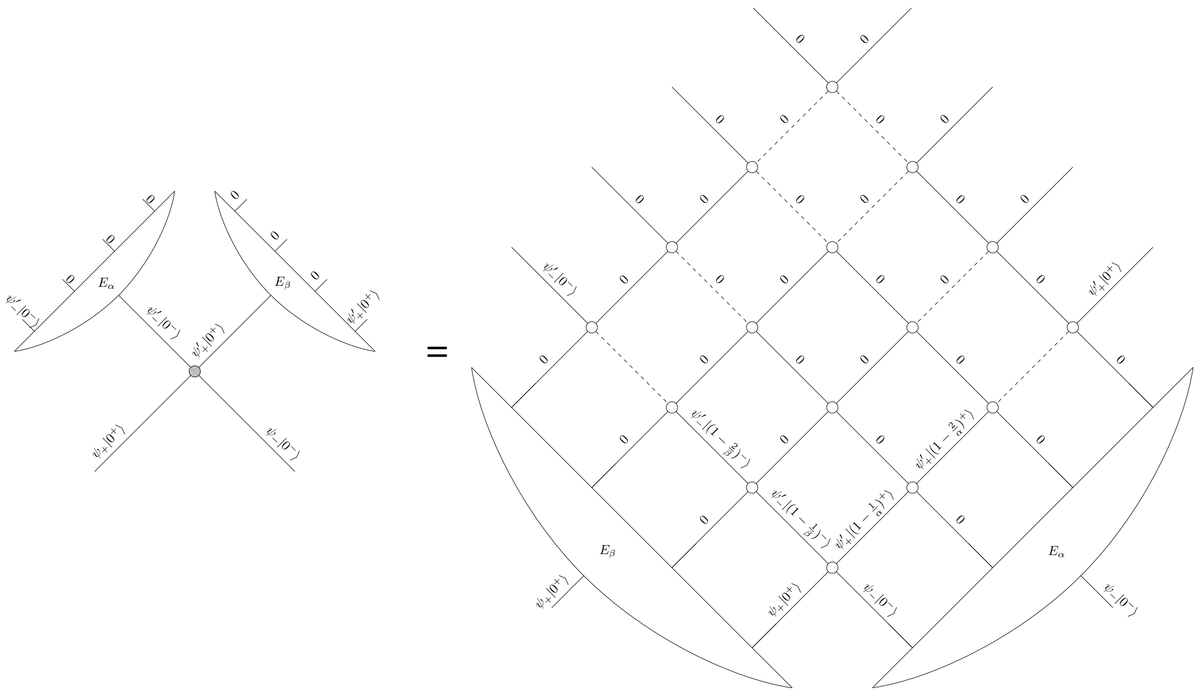


Figure 3.4.1: *Covariance of the Clock QW.* This is the transformation given by α, β of the Clock QW with parameters $p = 1, q = 1$.

3.4.2 Covariance

In order to prove covariance, we need to find isometries satisfying the equation expressed by Fig. 3.3.2(a). Let us consider isometries $E_\alpha : \mathcal{H}_C \to \bigoplus_\alpha \mathcal{H}_C$ defined by:

$$E_\alpha|h^s\rangle = (|h^s\rangle \oplus \overbrace{0 \oplus \cdots \oplus 0}^{\alpha-1\text{ times}}) \tag{3.4.4}$$

$$\tag{3.4.5}$$

(the Hilbert spaces in the direct sum are ordered from the bottom wire to the top one, as in remark 3.1). In Fig. 3.4.1 it is proved that this choice actually satisfies the covariance relation $\overline{E}C_{p,q} = \overline{C}_{p',q'}\,\overline{E}$, where the coin operator parameters have been rescaled as $p' = \alpha p$ and $q' = \beta q$. Intuitively, the Lorentz transformation rescales the fractional steps of the Clock QW by α (resp. β), while adding $\alpha - 1$ (resp. $\beta - 1$) more points to the lattice. In this way, the counter will reach 0 just at the end of the patch, as it did before the transformation.

3.4.3 Continuum limit of the Clock QW

The Clock QW does not have a continuum limit because its coin operator is not the identity in the limit $\varepsilon \to 0$. However, by appropriately sampling the spacetime points, it is possible to take the continuum limit of a solution of the Clock QW and show that it converges to a solution of the Dirac equation, subject to a Lorentz transform with parameters p, q. Indeed, the limit can be obtained as follows. First, we divide the spacetime in lightlike rectangular patches of dimension $p \times q$. Second, we choose as representative value for each patch the point where the interaction is non-trivial, averaged according to the dimensions of the rectangle:

$$\psi'(r,l) = \begin{pmatrix} \dfrac{\psi_+(\lfloor r/p \rfloor_\varepsilon , \lfloor l/q \rfloor_\varepsilon)}{\sqrt{q}} \\ \dfrac{\psi_-(\lfloor r/p \rfloor_\varepsilon , \lfloor l/q \rfloor_\varepsilon)}{\sqrt{p}} \end{pmatrix}.$$

Finally, by letting $\varepsilon \to 0$ we obtain

$$\psi'(r,l) = S\psi(r/p, l/q) \tag{3.4.6}$$

where now the r, l coordinates are to be intended as continuous.

Since ψ' is of course a solution of the Dirac equation (with a rescaled mass), this proves that the continuum limit of the Clock QW evolution, interpreted as described above, is again the Dirac equation itself.

3.4.4 Decoupling of the QW and the Klein-Gordon equation

The Clock QW does not have a proper continuum limit unless we exclude the intermediate computational steps. Still, as we shall prove in this section, its decoupled form *has* a proper limit, which turns out to be the Klein-Gordon Equation with a rescaled mass. By a decoupled form, we mean the scalar evolution law satisfied by each component of a vector field, individually (see [AF13]). In the following, we give the decoupled form of the Clock QW. The evolution matrix W is sparse and allows for decoupling by simple algebraic manipulations, leading to:

$$\left[T^{q+p} - a\tau^{-q}T^p - d\tau^p T^q + \det(C)\tau^{p-q}\right]\psi = 0 \tag{3.4.7}$$

(where $T = e^{\varepsilon\partial_t}$ and $\tau = e^{\varepsilon\partial_x}$). This is a discrete evolution law which gives the value of the current step depending on three previous time steps, namely the ones at $t = -p$, $t = -q$ and $t = -p - q$.

By expanding in ε the displacement operators and assuming that the coin operator verifies:

$$\det(C) = 1, \quad a = d = 1 + \frac{\varepsilon^2 m^2}{2} + O(\varepsilon^3) \tag{3.4.8}$$

(which is the case if $a = d = \cos(m\varepsilon)$) we obtain the continuum limit:

$$\left(\partial_t^2 - \partial_x^2 + \frac{m^2}{pq}\right)\psi = 0. \tag{3.4.9}$$

Up to redefinition of the mass $m' = m/\sqrt{pq}$, this is the Klein-Gordon Equation. This reinforces the interpretation of the Clock QW as model for a relativistic particle of mass m'.

3.5 The Clock QCA

One downside of the Clock QW is the fact that the dimension of the coin space varies according to the observer. Equipped with a formal, general notion of Lorentz transform and Lorentz covariance for QCA, we can now seek for an exactly covariant QCA of fixed, small, internal degree of freedom.

3.5.1 From the Clock QW to the Clock QCA

The idea of the Clock QW was to let the walker propagate during a number of steps to the right (resp. to the left), without spreading to the left (resp. to the right). In the absence of any other walker, this had to be performed with the help of an internal clock. In the context of QCA, however, the walker can be made to cross "keep going" signals instead.
The Clock QCA has wire dimension $d = 3$, with orthonormal basis $|q\rangle$, $|0\rangle$, $|1\rangle$. Both $|q\rangle$ and $|0\rangle$ should be understood as vacuum states, but of slightly different natures as we shall see next. $|1\rangle$ should be understood as the presence of a particle.
Thus, the Clock QCA has scattering unitary a 9×9 matrix U, which we can specify according to its action over the nine basis vectors. First we demand that the vacuum states be stable, i.e.

$$|q\rangle \otimes |q\rangle \mapsto |q\rangle \otimes |q\rangle, \tag{3.5.1a}$$
$$|q\rangle \otimes |0\rangle \mapsto |0\rangle \otimes |q\rangle, \tag{3.5.1b}$$
$$|0\rangle \otimes |q\rangle \mapsto |q\rangle \otimes |0\rangle, \tag{3.5.1c}$$
$$|0\rangle \otimes |0\rangle \mapsto |0\rangle \otimes |0\rangle. \tag{3.5.1d}$$

Second we demand that multiple walkers do not interact:

$$|1\rangle \otimes |1\rangle \mapsto |1\rangle \otimes |1\rangle. \tag{3.5.2}$$

Third we demand that the interaction between $|1\rangle$ and $|q\rangle$ be dictated by a massless Dirac QW, or "Weyl QW", i.e. the single walker goes straight ahead:

$$|1\rangle \otimes |q\rangle \mapsto |q\rangle \otimes |1\rangle, \tag{3.5.3a}$$
$$|q\rangle \otimes |1\rangle \mapsto |1\rangle \otimes |q\rangle. \tag{3.5.3b}$$

Last we demand that the interaction between $|1\rangle$ and $|0\rangle$ be dictated by:

$$|1\rangle \otimes |0\rangle \mapsto a(|0\rangle \otimes |1\rangle) + b(|1\rangle \otimes |0\rangle), \tag{3.5.4a}$$
$$|0\rangle \otimes |1\rangle \mapsto c(|0\rangle \otimes |1\rangle) + d(|1\rangle \otimes |0\rangle). \tag{3.5.4b}$$

This map is unitary provided that the 2×2 matrix C of coefficients $C_{11} = a$, $C_{12} = b$, $C_{21} = c$, $C_{22} = d$ is unitary. For instance we could choose, as for the Dirac QW, $a = d = \cos(m\varepsilon)$, $b = c = -\mathrm{i}\sin(m\varepsilon)$. The Clock QCA is covariant, even though its wire dimension is fixed and small, as we shall see.

3.5.2 Covariance of the Clock QCA

In order to give a precise meaning to the statement according to which the Clock QCA is covariant, we must specify our Lorentz transform. According to Section 3.3.2 we must provide a function f, which we take to be the identity, and an encoding $E_\alpha : \mathcal{H}_d \longrightarrow \mathcal{H}_d^{\otimes\alpha}$ which we take to be:

$$|a\rangle \mapsto |a\rangle \otimes \bigotimes_{\alpha-1} |q\rangle, \tag{3.5.5}$$

written from the bottom wire to the top wire as was the convention for QWs. The intuition is that the $(\alpha-1)$ ancillary wires are just there to stretch out this lightlike direction, but given that $|q\rangle$ interacts with no one, this stretching will remain innocuous to the physics of the QCA.

Let us prove that things work as planned:

$$\begin{aligned}
\overline{U}\,\overline{E}(|a\rangle \otimes |b\rangle) &= \left(\prod_{i=0\ldots\alpha-1, j=0\ldots\beta-1} U_{m'}\right) (|a\rangle^{0,0} \otimes \bigotimes_{i=1\ldots\alpha} |q\rangle^{i,0}) \otimes (|b\rangle^{0,0} \otimes \bigotimes_{j=1\ldots\beta} |q\rangle^{0,j}) \\
&= \left(\prod_{i=0\ldots\alpha-1, j=0\ldots\beta-1}^{(i,j)\neq(0,0)} U_{m'}\right) U(|a\rangle^{0,0} \otimes |b\rangle^{0,0}) \otimes \bigotimes_{i=1\ldots\alpha} |q\rangle^{i,0} \otimes \bigotimes_{j=1\ldots\beta} |q\rangle^{0,j}) \\
&= U(|a\rangle^{0,\beta-1} \otimes |b\rangle^{\alpha-1,0}) \otimes \bigotimes_{i=1\ldots\alpha} |q\rangle^{i,\beta-1} \otimes \bigotimes_{j=1\ldots\beta} |q\rangle^{\alpha-1,j} \\
&= \overline{E}U(|a\rangle \otimes |b\rangle).
\end{aligned} \tag{3.5.6}$$

Hence, the Clock QCA is Lorentz covariant. Notice that things would have worked equally well if E_α had placed $|a\rangle$ differently amongst the $|q\ldots\rangle$. It could even have spread out $|a\rangle$ evenly across the different positions, in a way that is more akin to the Lorentz transform for the Dirac QW.

3.6 Discussion of the physical interpretation

We formalized discrete Lorentz covariance as a form of commutativity: $\overline{E}C_m = \overline{C}_{m'}\overline{E}$. In the continuum, Lorentz covariance is not usually expressed as a commutation relation. However, consider a unitary representation of the Poincaré group: $U(a,\Lambda)\psi(x) = S(\Lambda)\psi(\Lambda^{-1}(x-a))$. Since the representation has to be homomorphic, one has:

$$U(0,\Lambda)U(a,\mathrm{id}) = U(\Lambda^{-1}a,\mathrm{id})U(0,\Lambda). \tag{3.6.1}$$

If a is along time, then $U(a,\mathrm{id})$ is the time evolution (analogous to the discrete, local C_m), and $U(\Lambda^{-1}a,\mathrm{id})$ the time evolution in the new frame (analogous to the discrete, rectangular patch $\overline{C}_{m'}$). Similarly, $U(0,\Lambda)$ in the continuous encoding (analogous to the discrete $\overline{E}$). Hence, the discrete Lorentz covariance condition is very much akin to the statement of the existence of a unitary representation of the Poincaré group, only with two added twists. First, it is expressed locally within lightlike rectangular patches of spacetime, which is always possible due to the boundedness of the speed of light, but seems more conveniently done in the discrete setting. Second, we do not look for a unitary representation but for an isometric representation, and crucially rely on covariance up to a mass rescaling under a conformal change of metric (aka scale covariance) of the evolutions of physics (as required by General Relativity), in order to fit the encoded ψ back on the grid.

In the continuum setting, the Lagrangian formulation of Lorentz covariance is often preferred to that based on the existence of a unitary representation of the Poincaré group. This is for practical reasons: it suffices to check that the Lagrangian is an invariant scalar in order to prove covariance, whereas exhibiting a unitary representation is not easy. It could be said that the discrete Lorentz covariance suffers precisely the same downside: it is not easy to see whether a QW or a QCA is Lorentz covariant. Yet, the downside is slightly diminished by the fact that $\overline{E}C_m = \overline{C}_{m'}\overline{E}$ is a local expression. Moreover, the fact that scale covariance enters early in the game, puts us on track of which QW or QCA will work. Intuitively, only those which can be rescaled in the sense of the renormalization group, favouring a lightlike direction over the other at will, are suitable. In this chapter we saw three mechanisms for implementing these lightlike stretchings: the first-order linear loss of the Dirac QW, the internal states of the Clock QW, and the quiescent signals of the Clock QCA. It is not clear to us whether there exists a fourth mechanism, which would not be a variant of those three.

3.7 Summary

In the context of QW and QCA, we have formalized a notion of discrete Lorentz transform of parameters α, β, which consists in replacing each spacetime point with a lightlike $\alpha \times \beta$ rectangular spacetime patch, $\overline{C}_{m'}\overline{E}$, where $\overline{E}$ is an isometric encoding, and $\overline{C}_{m'}$ is the repeated application of the unitary interaction $C_{m'}$ throughout the patch (see Fig. 3.2.2). We then formalized discrete Lorentz covariance as a form of commutativity: $\overline{E}C_m = \overline{C}_{m'}\overline{E}$. This commutation rule as well as the fact the E is isometric can be expressed diagrammatically in terms of a few local, circuit equivalence rules (see Fig. 3.3.2 and 3.3.3), à la [Coe10]. This simple diagrammatic theory allows for non-homogeneous Lorentz transforms (Fig. 3.3.6), which let you switch between non-inertial observers.

Chapter 4

Quantum walks in curved spacetime

In previous chapters we have seen that some QWs admit a continuum limit, leading to familiar PDEs (e.g. the Dirac equation), and thus provide us with discrete toy models of familiar particles (e.g. the electron). In this chapter, we study the continuum limit of a wide class of QWs, and show that it leads to an entire class of PDEs, encompassing the Hamiltonian form of the massive Dirac equation in $(1 + 1)$ curved spacetime. Therefore a certain QW, which we make explicit, provides us with a unitary discrete toy model of the electron as a test particle in curved spacetime, in spite of the fixed background lattice. Mathematically we have introduced two novel ingredients for taking the continuum limit of a QW, but which apply to any quantum cellular automata: encoding and grouping.

We proceed by first formally defining the model (Section 4.1). We then compute the conditions for the continuum limit to exist, and provide a complete parametrization of the QW operators in terms of the metric, in Section 4.2. Then we identify the continuum limit with the Dirac equation in curved spacetime, and validate the model with numerical simulations in Section 4.3. Finally, we discuss perspectives and related works in Section 4.4.

4.1 Introduction

4.1.1 From QWs to Paired QWs

Recall that usual one-dimensional QWs act on the space $\ell^2(\mathbb{Z}; \mathbb{C}^d \oplus \mathbb{C}^d)$, equal to the set of square summable sequences in the space $\bigoplus_{\mathbb{Z}}(\mathbb{C}^d \oplus \mathbb{C}^d)$. Often, the dimension of the internal degree of freedom is two, corresponding to $d = 1$. We denote $\psi(t)$ those functions taking a lattice position x into the $\mathbb{C}^{2d}$-vector $\psi^+(t, x) \oplus \psi^-(t, x)$, where each $\psi^\pm(t, x)$ is a $\mathbb{C}^d$-vector.

These QWs are induced by a local unitary W from $\mathbb{C}^{2d}$ to $\mathbb{C}^{2d}$ often referred to as the coin. Hence $c = 2d$ is often referred to as the coin dimension or internal degree of freedom of the walker. The reason why c must split as $d + d$ is because of the way W is wired: each $W(t, x)$ takes one half of $\psi(t, x - 1)$ (more precisely, its d upper components $\psi^+(t, x - 1)$) and half of $\psi(t, x + 1)$ (more precisely, its d lower components $\psi^-(t, x + 1)$) in order to produce $\psi(t + 1, x)$. This way the inputs and outputs of the different $W(t, x)$ are non-

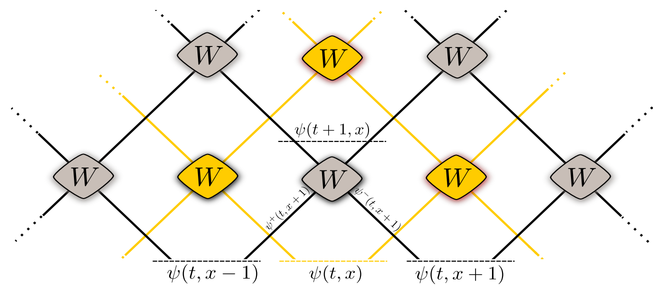


Figure 4.1.1: Usual QWs. Times goes upwards. Each site contains a $2d$-dimensional vector $\psi = \psi^+ \oplus \psi^-$. Each wire propagates the d-dimensional vector $\psi^\pm$. These interact via the $2d \times 2d$ unitary W. The circuit repeats infinitely across space and time. Notice that there are two light-like lattices evolving independently.

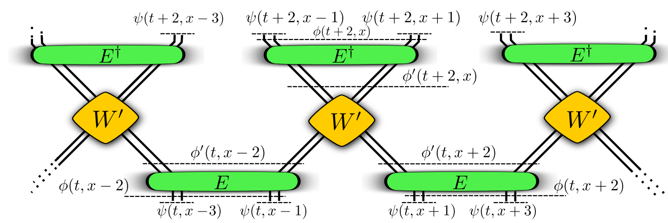


Figure 4.1.2: The input to a Paired QW is allowed to be encoded via a unitary E, and eventually decoded with $E^\dagger$.

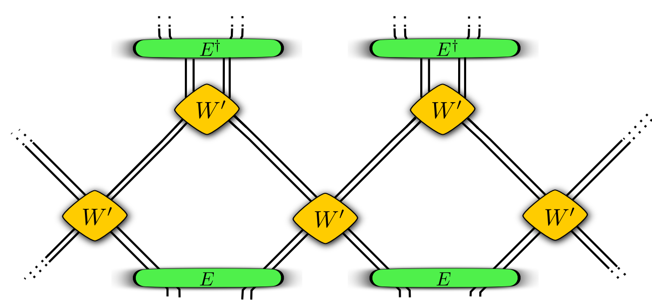


Figure 4.1.3: When the scheme is iterated, the decoding of the previous time-step cancels out with the encoding of the next time step. Thus the only relevant encoding/decoding are those of the initial input and final output. A Paired QW is therefore really just a QW, with a particular choice of initial conditions.

overlapping and they can be applied synchronously to generate the QW evolution over the full line, so that

$$U(t) := \bigoplus_{x\in\mathbb{Z}} W(t,x) \tag{4.1.1}$$

generates one time step of the QW (we remark that t indicates possible time dependence of the local unitaries; do not confuse $U(t)$ with the evolution operator from time 0 to time t).

It follows that usual QWs evolve two independent light-like lattices, as emphasized in

Fig. 4.1.1. On one of the light-like lattices, the evolution is given by

$$V(t) := \bigoplus_{x\in 2\mathbb{Z}} W(t,x) \text{ and } V(t+1) := \bigoplus_{x\in 2\mathbb{Z}+1} W(t+1,x). \tag{4.1.2}$$

whilst on the other lattice everything is shifted by 1 in position,

$$V(t) := \bigoplus_{x\in 2\mathbb{Z}+1} W(t,x) \text{ and } V(t+1) := \bigoplus_{x\in 2\mathbb{Z}} W(t+1,x). \tag{4.1.3}$$

Paired QWs arise as follows. Bunching up every $\psi(t,x-1)$ and $\psi(t,x+1)$ site into $\phi(t,x) = \psi(t,x-1) \oplus \psi(t,x+1)$, and applying a unitary encoding E to each bunch, we obtain $\phi'(t,x) = E\phi(t,x)$. We may now define a QW over the space $\bigoplus_{2\mathbb{Z}}(\mathbb{C}^{2d} \oplus \mathbb{C}^{2d})$ of these encoded bunches ϕ'. The local unitary W' will be from $\mathbb{C}^{4d}$ to $\mathbb{C}^{4d}$, and each $W'(t,x)$ will take one half of $\phi'(t,x-2)$ (more precisely, its $2d$ upper components) and half of $\phi(t,x+2)$ (more precisely, its $2d$ lower components) in order to produce $\phi'(t+2,x)$. The inputs and outputs of the different $W'(t,x)$ are again non-overlapping and they can be applied synchronously to generate the QW evolution over the full line,

$$U(t) := \bigoplus_{x\in 2\mathbb{Z}} W'(t,x). \tag{4.1.4}$$

In the end, each $\phi'(t+2,x)$ may be decoded as $\phi(t+2,x) = E^\dagger \phi'(t+2,x)$ and be reinterpreted as $\phi(t+2,x) = \psi(t+2,x-1) \oplus \psi(t+2,x+1)$. Clearly this Paired QW (pictured in Figs. 4.1.2 and 4.1.3) phrased in terms of ϕ' and $d' = 2d$ is no different from the usual QW definition right above. At least from a discrete point of view.

When looking for a continuum limit, a subtle difference arises. Indeed, say that the regular initial condition is given in terms of the fine-grained spacelike surface of $\psi(t)$, which is assumed to be smooth, i.e. $\psi(t,x) \approx \psi(t,x+1)$. Then the resulting $\phi(t)$ will be smooth both externally, i.e. $\phi(t,x) \approx \phi(t,x+1)$, and internally, i.e. $\phi(t,x) \approx \psi(t,x) \oplus \psi(t,x)$, which is not so usual to ask for. Similarly, $\phi'(t)$ will be smooth both externally, i.e. $\phi'(t,x) \approx \phi'(t,x+1)$ and internally, $\phi'(t,x) \approx E(\psi(t,x) \oplus \psi(t,x))$. It turns out that such reinforced regularity conditions are necessary for some Paired QWs to have a limit.

The next paragraph is to emphasize that Paired QWs, and their reinforced regularity assumptions, are not ad-hoc: they arise naturally when one performs spacetime grouping of QWs.

A natural example of Paired QW is provided by performing the spacetime grouping of a usual QW, an operation which we now explain. The spacetime grouping operation takes a QW over $\bigoplus_{\mathbb{Z}}(\mathbb{C}^d \oplus \mathbb{C}^d)$, with local unitary W into a Paired QW over $\bigoplus_{2\mathbb{Z}}(\mathbb{C}^{2d} \oplus \mathbb{C}^{2d})$, with local unitary W', as pictured in Fig. 4.1.4.

It is important to notice that if the initial condition was given by $\psi(t)$ for the original walk, the initial condition for the spacetime grouped QW is now given by the $\phi'(t,x) = E(x)\phi(t,x)$, and $\phi(t,x) = \psi(t,x-1) \oplus \psi(t,x+1)$, as pictured in Fig. 4.1.4 again. In the end, each $\phi'(t+2,x)$ may be decoded as $\phi(t+2,x) = E^\dagger(x)\phi'(t+2,x)$ and be reinterpreted as $\phi(t+2,x) = \psi(t+2,x-1) \oplus \psi(t+2,x+1)$. This spacetime grouping is reminiscent of the "stroboscopic" approach of [DMBD13, DMBD14], but has the advantage of mapping

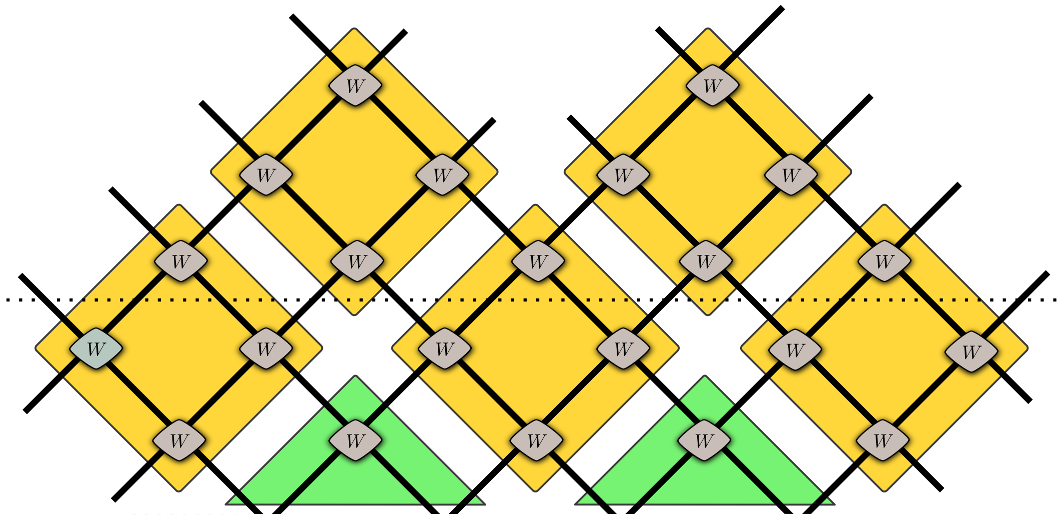


Figure 4.1.4: A Paired QW obtained by spacetime grouping of an ordinary QW. The green triangles define the appropriate encoding E, that relates the fine-grained input ψ with the coarsegrained input ϕ'. The dotted line indicates a $t+2$ space-like surface fine-grained output. This surface is recovered by undoing the triangles above these dotted line, which is the role of $E^\dagger$.

usual QWs into usual QWs of increased dimension.

4.1.2 Model definition

In this chapter, we study the continuum limits of Paired QWs (not necessarily arising from a spacetime grouping) for $d = 1$, systematically. Recall that for $d = 1$: $\psi(t)$ is in $\ell^2(\mathbb{Z};\mathbb{C}^2)$ and represents the 'physical' field; $\phi'(t)$ is in $\ell^2(\mathbb{Z};\mathbb{C}^4)$ and represents a paired, encoded version of it; W' is the 4×4 coin operator. For our purpose, it will be useful to redefine the bunching-up $\phi(t,x)$ as

$$\phi(t,x) := \begin{bmatrix} u(t,x) \\ d(t,x) \\ u'(t,x) \\ d'(t,x) \end{bmatrix}, \tag{4.1.5}$$

with

$$\begin{bmatrix} u(t,x) \\ u'(t,x) \end{bmatrix} = H \begin{bmatrix} \psi^+(t,x+1) \\ \psi^+(t,x-1) \end{bmatrix} \tag{4.1.6a}$$

$$\begin{bmatrix} d(t,x) \\ d'(t,x) \end{bmatrix} = H \begin{bmatrix} \psi^-(t,x+1) \\ \psi^-(t,x-1) \end{bmatrix} \tag{4.1.6b}$$

where $H = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}$ is the Hadamard matrix.

Notice that the $\psi(t,x)$ dependencies are the same as before, this is just a matter of applying a unitary pre-encoding. This convenient choice of basis is so that in the continuum limit, $u(t,x)$ becomes proportional to $\psi^+(t,x)$, whereas $u'(t,x)$ becomes proportional to the spatial derivative of $\psi^+(t,x)$.

Armed with those conventions on Paired QW, we can focus on how $\phi_{out} := \phi(t+2,x)$ gets computed, from $\phi_{in} := \phi(t,x-2) \oplus \phi(t,x+2)$. This $\mathbb{C}^4 \oplus \mathbb{C}^4$ to $\mathbb{C}^4$ function may be thought of as the local rule of a cellular automata with cells in $\mathbb{C}^4$. Its explicit formula is given by

$$\begin{aligned} G = E^\dagger(t+2,x)W'(t,x)(P' \oplus P) \\ (E(t,x-2) \oplus E(t,x+2)), \end{aligned} \tag{4.1.7}$$

where the 2×4 projectors P and P' pick-up the u, d (non-primed subspace) and u', d' (primed subspace) coordinates, respectively. Thus

$$\phi(t+2,x) = G(\phi(t,x-2) \oplus \phi(t,x+2)). \tag{4.1.8}$$

4.2 Continuum limit

From now on, we consider that t and x are continuous variables, and choose the same discretization step $\varepsilon \in \mathbb{R}^+$ for each coordinate. In particular note that, to first order in ε, we have that $u \simeq \sqrt{2}\psi^+$, $d \simeq \sqrt{2}\psi^-$, $u' \simeq \varepsilon\sqrt{2}\partial_x\psi^+$ and $d' \simeq \varepsilon\sqrt{2}\partial_x\psi^-$, see (4.1.6). To start investigating the continuum limit of the system defined by Eq. (4.1.7), we compute the expressions for the input and output.

The expansion of the input to first order in ε in terms of u, u', d, d' is

$$\phi_{in}(t,x) \simeq \begin{bmatrix} u \\ d \\ 0 \\ 0 \end{bmatrix} \oplus \begin{bmatrix} u \\ d \\ 0 \\ 0 \end{bmatrix} + \begin{bmatrix} -2u' \\ -2d' \\ u' \\ d' \end{bmatrix} \oplus \begin{bmatrix} 2u' \\ 2d' \\ u' \\ d' \end{bmatrix}. \tag{4.2.1}$$

We stress that u' and d' are themselves proportional to ε, hence the last term is proportional to ε.

The expansion of the output to first order in ε in terms of u, u', d, d' is

$$\phi_{out}(t,x) \simeq \begin{bmatrix} u \\ d \\ 0 \\ 0 \end{bmatrix} + \begin{bmatrix} 2\varepsilon\partial_t u \\ 2\varepsilon\partial_t d \\ u' \\ d' \end{bmatrix}. \tag{4.2.2}$$

Next we specify the structure of the walk and encoding operators. We shall assume, for simplicity, that the matrix elements of W and E are analytic functions of (t,x) and ε.

First, we set $W' := W^{(0)}e^{i\varepsilon\tilde{W}}$, with $W^{(0)}$ unitary and $\tilde{W}$ hermitian. This enforces the unitarity of W', and is without loss of generality, since only its expansion to first order in ε

matters:

$$W(t,x) \simeq W^{(0)}(t,x) + \mathrm{i}\varepsilon W^{(0)}(t,x)\tilde{W}(t,x). \tag{4.2.3}$$

Then, in a similar manner, we define $E := E^{(0)}e^{\mathrm{i}\varepsilon\tilde{E}}$, with $E^{(0)}$ unitary and $\tilde{E}$ hermitian. Hence, to first order in ε,

$$E(t,x) \simeq E^{(0)}(t,x) + \mathrm{i}\varepsilon E^{(0)}(t,x)\tilde{E}(t,x). \tag{4.2.4}$$

Here is some notation. Any matrix $A \in \mathbb{C}^{4\times 4}$ will be written in block form as $A = \begin{pmatrix} A_1 & A_3 \\ A_2 & A_4 \end{pmatrix}$, where $A_j \in \mathbb{C}^{2\times 2}$, $j = 1, \dots, 4$. Let $X = \sigma_x \otimes I$, $Y = \sigma_y \otimes I$ and $Z = \sigma_z \otimes I$, where $(\sigma_x, \sigma_y, \sigma_z)$ are the Pauli spin matrices.

Notice that, for any $A \in \mathbb{C}^{4\times 4}$, the following simplifications hold:

$$(P' \oplus P)(A \oplus A)(v \oplus v) = XAv \qquad \forall v \in \mathbb{C}^4 \tag{4.2.5}$$

and

$$(P' \oplus P)(A \oplus A)(-v \oplus v) = XZAv \qquad \forall v \in \mathbb{C}^4. \tag{4.2.6}$$

Next we develop the zeroth order and the first order expansion in ε of Eq. (4.1.7).

4.2.1 Zeroth order

For the left hand side we have just the zeroth order of (4.2.2), while for the right hand side there is only one term which does not contain ε, obtained multiplying all the zeroth order contributions. Hence

$$\begin{aligned} \begin{bmatrix} u \\ d \\ 0 \\ 0 \end{bmatrix} &= E^{(0)\dagger} W^{(0)} (P' \oplus P)(E^{(0)} \oplus E^{(0)}) \begin{bmatrix} u \\ d \\ 0 \\ 0 \end{bmatrix} \oplus \begin{bmatrix} u \\ d \\ 0 \\ 0 \end{bmatrix} \\ &= E^{(0)\dagger} W^{(0)} X E^{(0)} \begin{bmatrix} u \\ d \\ 0 \\ 0 \end{bmatrix}, \end{aligned} \tag{4.2.7}$$

where we used the simplification (4.2.5). The only non-trivial relations are

$$\begin{bmatrix} u \\ d \end{bmatrix} = \left(E^{(0)\dagger} W^{(0)} X E^{(0)}\right)_1 \begin{bmatrix} u \\ d \end{bmatrix} \tag{4.2.8}$$

$$\begin{bmatrix} 0 \\ 0 \end{bmatrix} = \left(E^{(0)\dagger} W^{(0)} X E^{(0)}\right)_2 \begin{bmatrix} u \\ d \end{bmatrix} \tag{4.2.9}$$

To satisfy (4.2.8) for arbitrary u and d, we must take the identity for block 1. Now, since the matrix in (4.2.7) is unitary, then both its rows and its columns must sum to one, thus the blocks 2 and 3 become zero, and (4.2.9) is automatically satisfied; we are left with the choice of an arbitrary unitary $U \in U(2)$ for block 4, to complete the matrix. Hence

$$E^{(0)\dagger} W^{(0)} X E^{(0)} = I \oplus U, \tag{4.2.10}$$

where the direct sum is respect to the non-primed subspace (spanned by the first two entries) and the primed subspace (spanned by the last two entries).

4.2.2 First order

For the left hand side we have just the first order of (4.2.2); note it contains time and space derivatives of $\psi^{\pm}$. For the right hand side we multiply and collect all possible combinations in which only one term contains ε. Then, after a long but straightforward calculation (see Appendix B.1 for the details), we get

$$\begin{aligned}\begin{bmatrix} 2\varepsilon\partial_t u \\ 2\varepsilon\partial_t d \\ u' \\ d' \end{bmatrix} &= (I \oplus U) \begin{bmatrix} 0 \\ 0 \\ u' \\ d' \end{bmatrix} + (I \oplus U) B \begin{bmatrix} 2u' \\ 2d' \\ 0 \\ 0 \end{bmatrix} \\ &+ \varepsilon \Big\{ (2N - \mathrm{i}\tilde{E})(I \oplus U) \\ &+ (I \oplus U)(\mathrm{i}\tilde{E} + 2M) + T \Big\} \begin{bmatrix} u \\ d \\ 0 \\ 0 \end{bmatrix}. \end{aligned} \tag{4.2.11}$$

with

$$B = E^{(0)\dagger} Z E^{(0)} \tag{4.2.12a}$$
$$N = (\partial_t E^{(0)\dagger}) E^{(0)} \tag{4.2.12b}$$
$$T = \mathrm{i} E^{(0)\dagger} W^{(0)} \tilde{W} X E^{(0)} \tag{4.2.12c}$$
$$M = E^{(0)\dagger} Z (\partial_x E^{(0)}). \tag{4.2.12d}$$

To deal with (4.2.11) we shall study separately what happens in the primed and in the non-primed subspaces.

4.2.3 Continuum limit equation

Projecting Eq. (4.2.11) on the non-primed subspace, we obtain an equation with time derivatives in the left hand side,

$$\begin{bmatrix} 2\varepsilon\partial_t u \\ 2\varepsilon\partial_t d \end{bmatrix} = B_1 \begin{bmatrix} 2u' \\ 2d' \end{bmatrix} + \varepsilon(2N_1 + T_1 + 2M_1) \begin{bmatrix} u \\ d \end{bmatrix}. \tag{4.2.13}$$

Switching to the original $\psi^{\pm}(t,x)$ coordinates, and writing $\psi(t,x) = [\psi^+(t,x), \psi^-(t,x)]^\mathsf{T}$,

$$\partial_t \psi(t,x) = B_1 \partial_x \psi(t,x) + \left(N_1 + \frac{T_1}{2} + M_1\right)\psi(t,x). \tag{4.2.14}$$

From (4.2.12a), applying Leibniz rule and using (4.2.12d) we have[1]

$$\partial_x B = M + M^\dagger = 2\Re M. \tag{4.2.15}$$

From (4.2.12b), the unitarity of $E^{(0)}$ implies that N is skew-hermitian,

$$N^\dagger = -N. \tag{4.2.16}$$

From (4.2.12c),

$$\begin{aligned} T &= \mathrm{i}E^{(0)\dagger}W^{(0)}\tilde{W}XE^{(0)} && (4.2.17)\\ &= \mathrm{i}E^{(0)\dagger}W^{(0)}XE^{(0)}E^{(0)\dagger}X\tilde{W}XE^{(0)} && (4.2.18)\\ &= \mathrm{i}(I\oplus U)E^{(0)\dagger}X\tilde{W}XE^{(0)}, && (4.2.19)\end{aligned}$$

where we used the zeroth order condition (4.2.10). Inverting,

$$\mathrm{i}E^{(0)\dagger}X\tilde{W}XE^{(0)} = (I\oplus U^\dagger)T = \begin{pmatrix} T_1 & T_3 \\ U^\dagger T_2 & U^\dagger T_4 \end{pmatrix}. \tag{4.2.20}$$

Since the left hand term is skew-hermitian we have that

$$\begin{aligned} T_1^\dagger &= -T_1 && (4.2.21a)\\ T_3 &= -T_2^\dagger U && (4.2.21b)\\ T_4^\dagger U &= -U^\dagger T_4. && (4.2.21c)\end{aligned}$$

Therefore, by spliting M_1 into its hermitian and skew-hermitian parts, and using equations (4.2.15), (4.2.16) and (4.2.21a), the continuum limit has the general form

$$\partial_t \psi(t,x) = B_1 \partial_x \psi(t,x) + \frac{1}{2}\partial_x B_1 \psi(t,x) + \mathrm{i}C\psi(t,x). \tag{4.2.22}$$

where C is an hermitian matrix defined by

$$\mathrm{i}C = N_1 + \frac{T_1}{2} + \mathrm{i}\Im M_1. \tag{4.2.23}$$

[1]Recall that if $A \in \mathbb{C}^{n\times n}$, its real and imaginary parts are $\Re A := \frac{1}{2}(A + A^\dagger)$ and $\Im A := \frac{1}{2\mathrm{i}}(A - A^\dagger)$, respectively.

4.2.4 Compatibility constraints

Projecting Eq. (4.2.11) onto the primed subspace, gives

$$\begin{aligned}\begin{bmatrix}u'\\d'\end{bmatrix} = U\begin{bmatrix}u'\\d'\end{bmatrix} + 2UB_2\begin{bmatrix}u'\\d'\end{bmatrix} + \varepsilon\Big(2N_2 - \mathrm{i}\tilde{E}_2 \\ + \mathrm{i}U\tilde{E}_2 + 2UM_2 + T_2\Big)\begin{bmatrix}u\\d\end{bmatrix}.\end{aligned} \tag{4.2.24}$$

Eq. (4.2.24) does not involve time derivatives. Therefore, these equations must be understood as constraints. Where do these come from? Recall that the aimed continuum limit equation (6.1.1) is over a $\mathbb{C}^2$ field, but the QW employed is over the $\mathbb{C}^4$ field obtained by pairing it. Thus, the $\mathbb{C}^4$ field as some internal smoothness initially, which the QW must preserve. More precisely, in order to have nontrivial, time-dependent solutions, the coeffients of $[u, v]^\mathsf{T}$ and $[u', v']^\mathsf{T}$ must vanish separately:

$$\begin{cases} U(I + 2B_2) = I, & \text{(4.2.25a)}\\ 2N_2 - \mathrm{i}(I - U)\tilde{E}_2 + 2UM_2 + T_2 = 0. & \text{(4.2.25b)}\end{cases}$$

4.2.5 Existence of solutions

Up to now we have determined the continuum limit, provided that the constraints (4.2.25a)-(4.2.25b) are satisfied. In this section we show that, given any hermitian B_1 and C, there are indeed compatible choices of W and E.

The strategy is the following. First we show that B_1 along with constraint (4.2.25a) determines the zeroth order part of E and W'. Then, using C and (4.2.25b) we complete the solution determining the first order terms.

4.2.5.1 Determination of B and U

Consider the spectral decomposition $B_1 = VDV^\dagger$, $D = \mathrm{diag}\{d_1, d_2\}$. In Appendix B.2 we show that Eq. (4.2.12a) implies that d_1, d_2 must belong to the interval $[-1, 1]$, and provide the general form of B given B_1 (see section 4.3 for a discussion about the eigenvalue constraint). Here we just pick one particular solution, namely

$$B = \begin{pmatrix} V^\dagger & 0\\ 0 & V^\dagger\end{pmatrix}\overline{B}\begin{pmatrix} V & 0\\ 0 & V\end{pmatrix}, \tag{4.2.26}$$

where $\overline{B}$ is

$$\overline{B} = \begin{pmatrix} d_1 & 0 & -\lambda_1 e^{\mathrm{i}\eta_1} & 0\\ 0 & d_2 & 0 & -\lambda_2 e^{\mathrm{i}\eta_2}\\ -\lambda_1 e^{-\mathrm{i}\eta_1} & 0 & -d_1 & 0\\ 0 & -\lambda_2 e^{-\mathrm{i}\eta_2} & 0 & -d_2\end{pmatrix}, \tag{4.2.27}$$

with $\lambda_i = \sqrt{1 - d_i^2}$, $\sin\eta_i = \pm|d_i|$, $-\pi/2 < \eta_i < \pi/2$, $i \in \{1, 2\}$.

Note that U is now fixed by Eq. (4.2.25a).

4.2.5.2 Determination of $E^{(0)}$ and $W^{(0)}$

From Eq. (4.2.12a) we know that $E^{\dagger(0)}$ diagonalizes B. Then, its columns can be chosen to be any complete set of normalized eigenvectors of B. More generally, we could take $\begin{pmatrix} R & 0 \\ 0 & S \end{pmatrix} E^{(0)}$ for arbitrary $R, S \in U(2)$, because of the degeneracy of order two for each eigenvalue $+1$, -1.

For the special case of $\overline{B}$ in Eq. (4.2.27), we can give an explicit solution $\overline{E}^{(0)}$,

$$\overline{E}^{(0)} = \frac{1}{\sqrt{2}} \begin{pmatrix} \nu_1^+ & 0 & -\nu_1^- e^{\mathrm{i}\eta_1} & 0 \\ 0 & \nu_2^+ & 0 & -\nu_2^- e^{\mathrm{i}\eta_2} \\ \nu_1^- & 0 & \nu_1^+ e^{\mathrm{i}\eta_1} & 0 \\ 0 & \nu_2^- & 0 & \nu_2^+ e^{\mathrm{i}\eta_2} \end{pmatrix}, \tag{4.2.28}$$

where $\nu_i^\pm = \sqrt{1 \pm d_i}$, $i \in \{1, 2\}$.

Once $E^{(0)}$ is known, we can compute $W^{(0)}$ from (4.2.10).

4.2.5.3 Determination of $\tilde{E}$ and $\tilde{W}$

The choice of $E^{(0)}$ determines N_1 and M_1 via Eqs. (4.2.12b) and (4.2.12d), so T_1 is fixed by Eq. (4.2.23) once we choose C.

Since $\tilde{E}$ does not appear in the continuum limit, without loss of generality we can take $\tilde{E} = 0$. In this way T_2 is fixed by the contraint (4.2.25b).

In order to complete T it is now sufficient to take $T_4 = 0$, and T_3 from (4.2.21b). Finally, from (4.2.20) we find $\tilde{W}$,

$$\tilde{W} = -\mathrm{i} X E^{(0)} (I \oplus U^\dagger) T E^{(0)\dagger} X. \tag{4.2.29}$$

4.2.6 Recap

We have shown that the continuum limit of our model is given by Eq. (6.1.1). Moreover, we provided a procedure to obtain the parameters of the quantum walk, namely the unitaries W' and E, given a pair of hermitian matrices B_1 and C, possibly spacetime dependent. We remark that the choices made in the procedure are in general not unique. In the emergent continuum limit, different choices of E, W' lead in general to the same equation.

Notice also that the minimal coupling (e.g. electric field) is already considered in the parameter C.

The whole procedure was programmed in `sagemath`, and made available in the author's webpage.

4.3 Recovering the Dirac equation

On a spacetime with metric tensor $g_{\mu\nu}$ and in the absence of external fields, the Dirac equation in Hamiltonian form [DOT62] is $\mathrm{i}\partial_t\psi = H_D\psi$, with

$$H_D = -\mathrm{i}\left(\alpha\frac{e_1^1}{e_0^0} + e_0^1\right)\partial_x - \frac{\mathrm{i}}{2}\partial_x\left(\alpha\frac{e_1^1}{e_0^0} + e_0^1\right) + \frac{m}{e_0^0}\beta,$$

where m is the mass and α, β are matrices satisfying $\alpha^2 = \beta^2 = I$, $\alpha\beta + \beta\alpha = 0$ (here and in the following we assume natural units, $\hbar = c = G = 1$). Here $e_a^\mu(t,x)$ are the *dyads*, which are related to the metric via $g_{\mu\nu}(t,x)e_a^\mu(t,x)e_b^\nu(t,x) = \eta_{ab}$, where η_{ab} is the Minkowski metric.

Making the identification with the continuum limit of our discrete model, Eq. (6.1.1), we find

$$B_1 = -\frac{e_1^1}{e_0^0}\alpha - e_0^1 \tag{4.3.1}$$

$$C = -\frac{m}{e_0^0}\beta. \tag{4.3.2}$$

These equations allow to find the QW parameters, associated to a given metric. The constraint that the eigenvalues of B_1 are $d_{1,2} \in [-1,1]$ represents the finite speed of propagation on the lattice. In practice, for any region of spacetime where the metric field is bounded, it is possible to rescale the coordinates in such a way that the physical lightcones are inside the "causal lightcones" of the discrete model.

For instance, we can specialize the previous considerations to the case of the Schwarzschild metric, whose radial part is

$$ds^2 = (1-2M/x)dt^2 - (1-2M/x)^{-1}dx^2, \tag{4.3.3}$$

where x corresponds to the radial coordinate [2]. Choosing the chiral representation [Tha92], namely $\alpha = \sigma_z$ and $\beta = \sigma_x$, we have

$$B_1 = -\left(1 - \frac{2M}{x}\right)\sigma_z \tag{4.3.4}$$

$$C = -m\left(1 - \frac{2M}{x}\right)^{1/2}\sigma_x. \tag{4.3.5}$$

A simulation for a particle in the Schwarzschild metric is shown in Fig. 4.3.1. Again the `sagemath` program which converts any metric into the corresponding QW, and produces such simulations, is available at the author's webpage.

[2] In this case the dyads are $e_0^0 = (1-2M/x)^{-1/2}$, $e_1^1 = (1-2M/x)^{1/2}$, and $e_1^0 = e_0^1 = 0$.

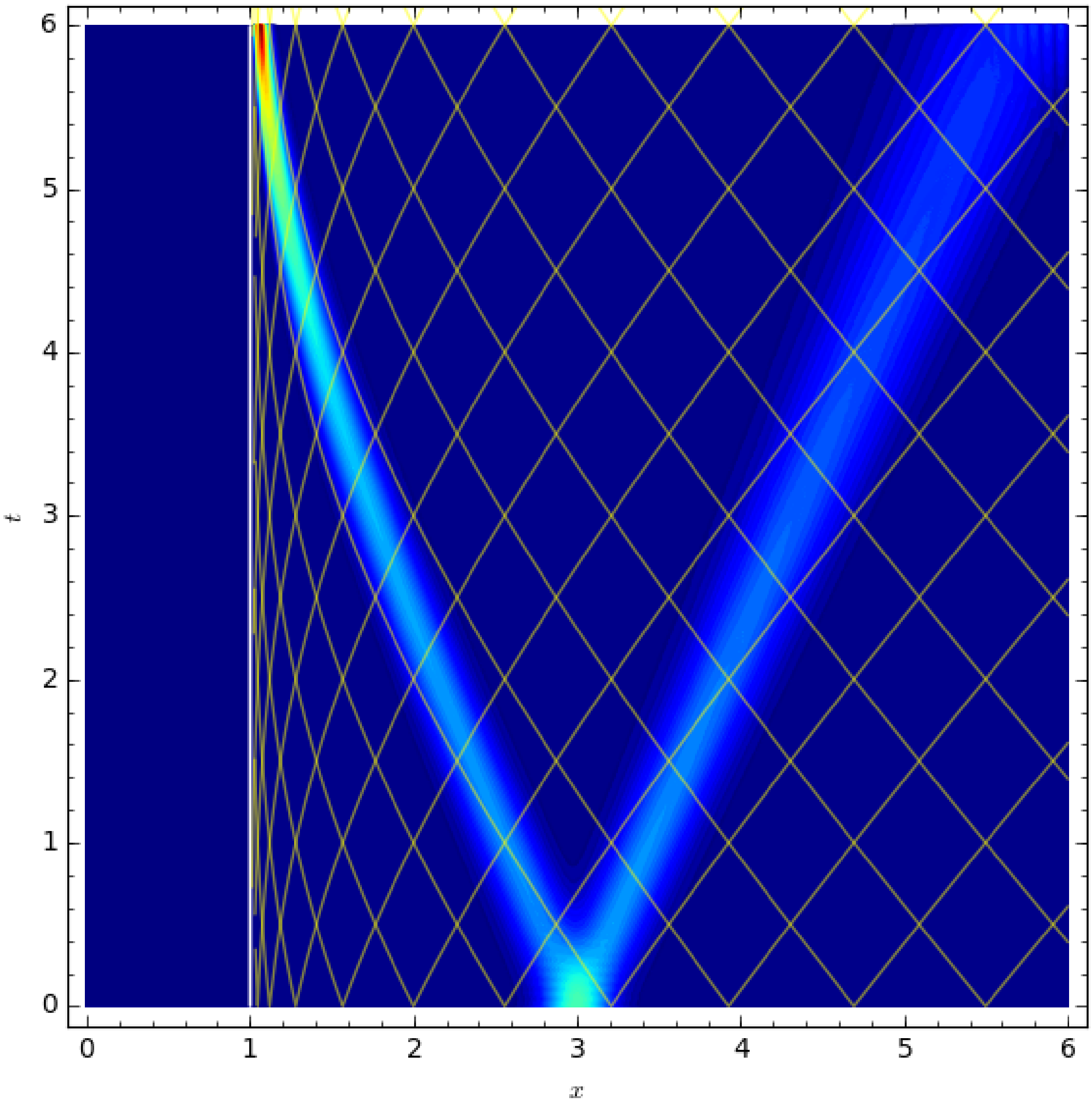


Figure 4.3.1: Simulation of the Paired QW for the Schwarzschild metric with mass parameter $M = 0.5$. We plot the probability density for a particle with initial condition given by a gaussian wavepacket $\phi(x) \propto \int e^{-(p-p_0)^2/(2\sigma^2)+\mathrm{i}(x-x_0)p}\,(u_+(p) + u_-(p))\,dp$ where $x_0 = 3.0$, $p_0 = 50$, $\sigma = 1.56$ and $u_\pm$ are the eigenvectors of the free Dirac Hamiltonian $H_0 = \alpha\hat{p} + m\beta$. The mass of the particle is $m = 50$. For comparison, we show in yellow a grid of null geodesics. The lattice spacing is $\varepsilon = 5 \times 10^{-5}$.

4.4 Summary

In summary, we have constructed a QW, i.e. a strictly unitary, causal, local evolution, which implements the idea of "encoding-evolution-decoding" of the discrete dynamics, defined in Eq. (4.1.8). We have found that Paired QWs with $d = 1$ admit as continuum limit all PDEs of the form (6.1.1). This class encompasses the Hamiltonian form of the Dirac equation in curved spacetime, together with an electromagnetic field.

In this model, curvature is effectively implemented by a collection of spacetime dependent local unitaries (namely, the unitary operators $E(t, x)$ and $W'(t, x)$), which are distributed over a fixed background lattice, and whose purpose is to drive the particle according to the metric.

Chapter 5

Spectral properties of interacting quantum walks

DETERMINATION of discrete spectrum, i.e. isolated eigenvalues of finite algebraic multiplicity, is a recurrent problem in mathematical physics. Its importance lies on the fact that the presence of eigenvalues reveals that the system has *bound states*, that is, states which tend to be localized in some region of space. Although the analytic computation of the full spectrum of an operator is sometimes possible, e.g. the hydrogen atom, most of the time in physics and chemistry it is definitely not the case. However much physical insight is obtained with the functional analysis approach, i.e. through spectral analysis[1]. For instance, it serves to provide information about velocity of convergence of the eigenvalues towards some accumulation point (as Lieb-Thirring estimates), or to unravel existence conditions that can be checked numerically.

5.1 Introduction

The aim of this chapter is to perform a spectral analysis of the two-particle sector of a QCA, which we call an IQW. We collect in Appendices C.1 and C.2 the background on distribution theory and Hilbert space that serves as a complement for the mathematics. The approach of this chapter is quite different from the rest of the thesis: instead of focusing on the continuum limit, we are mainly interested in the discrete dynamical system itself, i.e. in QWs models *per se*. In this sense the QW is seen as the generator of "spreading" of an initial state driven by the iterates of a unitary operator, quoting [DFV14]. Let us begin with a recap.

[1] A standard reference is [RS80]; another valuable reference for a rigorous approach to quantum mechanics is [Tes14].

5.1.1 Recap

Let $\mathcal{H}_1 = \ell^2(\mathbb{Z}) \otimes \mathbb{C}^2$ be the Hilbert space of $\mathbb{C}^2$-valued doubly infinite square summable sequences, with inner product

$$\langle \psi, \varphi \rangle = \sum_{x\in\mathbb{Z}} \psi^\dagger(x)\varphi(x). \tag{5.1.1}$$

Here $\mathcal{H}_1$ represents the abstract state space of a lattice model of a quantum particle with an internal two-dimensional degree of freedom.

According to quantum mechanics, the n-particle sector is obtained by tensoring $\mathcal{H}_1$ with itself, that is, considering $\mathcal{H}_n = \mathcal{H}_1^{\otimes n}$. A quantum walk (QW) on $\mathcal{H}_n$ is defined as the operator

$$\mathcal{U}_0 = \bigotimes_{j=1}^{n} (S_j \cdot (I_\mathbb{Z} \otimes C_j)), \tag{5.1.2}$$

where S_j are nearest-neighbour translation operators conditional on the internal state, i.e. $S_j|x_j, \sigma_j\rangle = |x_j + \sigma_j, \sigma_j\rangle$ for all $x_j \in \mathbb{Z}$, $\sigma_j \in \{\pm 1\}$, where $I_\mathbb{Z}$ denotes the identity operator in the sequence space $\ell^2(\mathbb{Z})$ and where $C_j \in U(2)$ are unitary matrices with constant coefficients.

In this chapter we consider an interacting QW (IQW) of two particles,

$$\mathcal{U} = \mathcal{U}_0\mathcal{V}, \tag{5.1.3}$$

with $\mathcal{U}_0$ defined as in (5.1.2), fixing $n = 2$, coupled to an interaction operator $\mathcal{V}$, defined as the multiplication by a position (x) and spin (σ) dependent unitary matrix,

$$(\mathcal{V}\psi)(x_1, x_2) = V(x_1, x_2)\psi(x_1, x_2), \qquad V \in U(4). \tag{5.1.4}$$

Our main goal is to analyse the existence and location of the discrete spectrum of $\mathcal{U}$ if we assume physically motivated hypothesis at increasing relative separation of the particles $|x_1 - x_2| \to \infty$.

5.1.2 Notation

The direct[2] space is discrete, hence the letters x, x_1, x_2, always denote discrete-valued (in general integer) variables. We use $|x_1, x_2, \sigma_1, \sigma_2\rangle$ to denote the elements of the basis of $\mathcal{H}_2 = \mathcal{H}_1 \otimes \mathcal{H}_1$, with $\sigma_1, \sigma_2 \in \{\pm 1\}$. Here $|x_1, \sigma_1\rangle$ corresponds to the first copy of $\mathcal{H}_1$ while $|x_2, \sigma_2\rangle$ corresponds to the second copy of $\mathcal{H}_1$. Consequently, wavefunctions $\psi \in \mathcal{H}_2$ are written as

$$\psi = \sum_{x_1, x_2 \in\mathbb{Z}} \psi(x_1, x_2)|x_1, x_2\rangle, \tag{5.1.5}$$

[2] We sometimes use the jargon of condensed matter physics, with *direct* (resp. *reciprocal*) meaning the x_1, x_2 space (resp. the space of the Fourier transform in the variables k_1, k_2).

and where $\psi(x_1, x_2) \in \mathbb{C}^4$ is

$$\psi(x_1, x_2) = \sum_{\sigma_1, \sigma_2} \psi^{\sigma_1 \sigma_2}(x_1, x_2) |\sigma_1, \sigma_2\rangle. \tag{5.1.6}$$

Let $\mathbb{N}_0 = \mathbb{Z}_+ \cup \{0\}$, with $\mathbb{Z}_+$ being the set of positive integers. Let $\mathbb{T} = \mathbb{R}/2\pi\mathbb{Z}$ be the (one-dimensional) torus, which we identify with the segment $[-\pi, \pi]$. For vectors $x \in \mathbb{Z}^n$, we note $\langle x \rangle = (1 + ||x||^2)^{1/2}$, $||x||$ being its Euclidean norm. A multi-index is an n-tuple $\alpha = (\alpha_1, \dots, \alpha_n) \in \mathbb{N}_0^n$, and its order is $|\alpha| = \alpha_1 + \dots + \alpha_n$, and $x^\alpha = x_1^{\alpha_1} \cdots x_n^{\alpha_n}$. Partial differentiation is written $D^\alpha = D_1^{\alpha_1} \cdots D_n^{\alpha_n}$, where $D_j = \frac{1}{\mathrm{i}} \partial_j$ for $j = 1, \dots, n$, and translation of a function f is denoted $(\tau_{x_0} f)(x) = f(x - x_0)$.

Given a function $f : I \to \mathbb{C}$, $I \subset \mathbb{R}$, $\Re(f(k))$ and $\Im(f(k))$ denote the real and imaginary part of $f(k)$ respectively, and $\operatorname{Im} f$ denotes its image, i.e. $\operatorname{Im} f = \{f(k) : k \in I\}$.

Finally, we write $A \in \mathcal{M}_n(X)$ for A an $n \times n$ matrix whose elements take values on the vector space X, and the identity is denoted I_n. With $||A||_F$ we denote the Frobenius norm of matrix, that is, $||A||_F = \sqrt{\operatorname{Tr}(A^\dagger A)}$ where $A^\dagger$ denotes the conjugate transpose of A, i.e. $\overline{A}^{\mathrm{T}}$.

5.1.3 Assumptions on the interaction

Some physically motivated notions are in order. For simplicity of notation we associate the interaction operator $\mathcal{V} \in \mathcal{L}(\mathcal{H}_2)$ acting as in Eq. (5.1.4) with the sequence of matrices defining it, that is, with $\{V(x_1, x_2) \in \mathcal{M}_4(\mathbb{C}) : x_1, x_2 \in \mathbb{Z}\}$.

Definition 5.1. *An IQW $\mathcal{U} = \mathcal{U}_0 \mathcal{V}$ is said to be:*

- unitary *if $V(x_1, x_2) \in U(4)$ for all $x_1, x_2 \in \mathbb{Z}$.*
- symmetric *if $V(x_1, x_2) = V(x_2, x_1)$ for all $x_1, x_2 \in \mathbb{Z}$.*
- radial *if $V(x_1, x_2) = V(|x_1 - x_2|)$ for all $x_1, x_2 \in \mathbb{Z}$.*
- vanishing at infinity *if $||I_4 - V(x_1, x_2)||_F \to 0$ as $|x_1 - x_2| \to \infty$.*
- p-summable *if $\sum_{x_1, x_2 \in \mathbb{Z}} ||I_4 - V(x_1, x_2)||_F^p < \infty$ for some $p \geq 1$.*
- finite range *if there exists $N > 0$ such that $V(x_1, x_2) = I_4$ for all x_1, x_2 such that $\sqrt{x_1^2 + x_2^2} \geq N$.*

In this chapter we consider the joint hypothesis:

(H0) $\mathcal{V}$ is vanishing at infinity, unitary, and radial (hence symmetric).

Note that under **(H0)**, the walk operator $\mathcal{U} = \mathcal{U}_0 \mathcal{V}$ is a unitary operator in $\mathcal{H}_2$. Moreover, $\mathcal{V}$ only depends on the relative coordinate $x := x_1 - x_2 \in \mathbb{Z}$. The difference of the interaction with respect to its value at infinity at relative position $x \in \mathbb{Z}$ is denoted

$$D(x) = I_4 - V(x) \in \mathcal{M}_4(\mathbb{C}), \quad \text{with norm } \Delta(x) = ||D(x)||_F. \tag{5.1.7}$$

In this chapter we study the existence and location of discrete spectra of the IQW if we assume additional p-summability of the interaction, i.e. finiteness of weighted sums

$$\sum_{x=1}^{\infty} \Delta^p(x) < \infty \tag{5.1.8}$$

for some $p \geq 1$. In our analysis, an important role is played by interactions which are *trace-class*, meaning that for $p = 1$, (5.1.8) holds.

5.1.4 Chapter outline

The rest of the chapter is organized as follows. In Section 5.2, we perform the reduction of the two-particle case to the relative problem. This is essential because all the subsequent analysis relies on decoupling the relative with the total momentum coordinates. In Section 5.3, we study in detail the spectral properties of the free QW, for arbitrary choices of parameters. This allows to understand what kind of phenomena to expect when the interaction is "switched on". We begin the spectral analysis of the perturbed QW in Section 5.4, where we derive a condition for the absence of singular continuous spectrum. In Section 5.5 we find some Lieb-Thirring type estimates for the distribution of eigenvalues. In Section 5.6 we address the abstract eigenvalue problem, and we provide its formal solution in terms of a system of Fredholm integral equations with a compatibility constraint. In Section 5.7 we revisit the contact interaction and propose models of long-range interactions that may depend on the spin components, for which the approach can be applied. We summarize our results in Section 5.8.

5.1.5 Related works

The extension of the discrete-time QW to multiple walkers was first studied by Omar et al. in 2004 [OPSB06]. They studied a two-particle QW on the line, and proved that coin entanglement induces spatial correlations between the spatial degrees of freedom. In their case the QW is *non-interacting*, in the sense that the coins are homogeneous. This subject was pursued further in [BW11, ŠBK$^+$11, LZG$^+$13], and physically implemented in [SGR$^+$12]. One should recall that the non-interacting case is not trivial in quantum mechanics. Indeed, a system with multiple particles –even non-interacting– presents new interesting features that depart from classical mechanics: there is entanglement and there are quantum statistical aspects, such as distinguishability.

Besides, researchers have studied non-homogeneous QWs with a "defect", i.e. assuming that the coin operator is everywhere the same and distinct at a fixed position. Two different approaches are the method of CMV matrices [KN07] (since the QW matrix is naturally CMV-shaped), see [CGMV12], and the method of generating functions [KŁS13]. Non-homogeneous quantum walks have also been studied under periodic coins [LS09, SK10], and shown numerically that in some circumstances the spectrum has behaviour similar to the self-simliar Hofstadter butterfly [Hof76].

Finally, in [AAM$^+$12] they consider the non-homogeneity of the coin as an interaction.

In particular, they study the spectrum of an IQW with a zero range interaction. In this case $V(0) = e^{\mathrm{i}g} I_4$, and I_4 otherwise. They prove the presence of eigenvalues in the gaps of the continuous spectrum, interpreted as molecular binding. This phenomenon manifests itself in the joint probability distributions as peaks wich are close to each other even after a long time, and the wave-function decays exponentially in the relative position of the two particles.

5.2 Reduction to the relative problem

The main goal of this section is to show that under hypothesis **(H0)**, the dynamics is reduced to a one-particle problem in the relative coordinate in momentum space. The reduction is accomplished exploiting the symmetry properties of the IQW.

We collect in Appendix C.1 a review of distribution theory on the n-dimensional Torus $\mathbb{T}^n$, with the background needed for this section.

5.2.1 States in the relative and total momentum representation

Recall that $\mathcal{H}_2 = \ell^2(\mathbb{Z}^2) \otimes \mathbb{C}^4$, and let $\hat{\mathcal{H}}_2 = L^2(\mathbb{T}^2) \otimes \mathbb{C}^4$. By Fourier transformation on $L^2(\mathbb{T}^n)$, $\mathcal{F} : \mathcal{H}_2 \to \hat{\mathcal{H}}_2 : \psi \mapsto \hat{\psi}$,

$$\hat{\psi} = \frac{1}{(2\pi)^2} \int_{\mathbb{T}^2} \hat{\psi}(k_1, k_2) |k_1, k_2\rangle \mathrm{d}k_1 \mathrm{d}k_2, \tag{5.2.1}$$

where

$$\hat{\psi}(k_1, k_2) = \sum_{x_1, x_2} e^{-\mathrm{i}(k_1 x_1 + k_2 x_2)} \psi(x_1, x_2), \qquad k_1, k_2 \in [-\pi, \pi]. \tag{5.2.2}$$

The inverse transformation is given by

$$\psi(x_1, x_2) = \frac{1}{(2\pi)^2} \int_{\mathbb{T}^2} e^{\mathrm{i}(k_1 x_1 + k_2 x_2)} \hat{\psi}(k_1, k_2) \mathrm{d}k_1 \mathrm{d}k_2. \tag{5.2.3}$$

Let the *relative momentum* k, and *total momentum* p, be defined by the map

$$(k_1, k_2) \mapsto (k, p) = \left(\frac{k_1 - k_2}{2}, k_1 + k_2 \right). \tag{5.2.4}$$

Note that

$$k_1 = \frac{p}{2} + k, \qquad k_2 = \frac{p}{2} - k, \tag{5.2.5}$$

and

$$k_1 x_1 + k_2 x_2 = sp/2 + kd, \qquad \text{where } s = x_1 + x_2, \text{ and } d = x_1 - x_2. \tag{5.2.6}$$

Remark 5.1. We follow [AAM+12] for the map (5.2.4). The extra factor of $1/2$ is convenient because it allows to assume that both pairs of variables (k_1, k_2) and (k, p) run through $[-\pi, \pi]^2$, by folding appropriately those zones of the (k_1, k_2) graph which make p to lie outside the square $[-\pi,\pi]^2$, see Fig. 5.2.1[3]. Formula (5.2.6) also has the property that its dependence in k will make appear a factor $e^{\mathrm{i}kd}$, and this is useful because, as we show in the next subsection, it allows to identify a Fourier series in the relative coordinate.

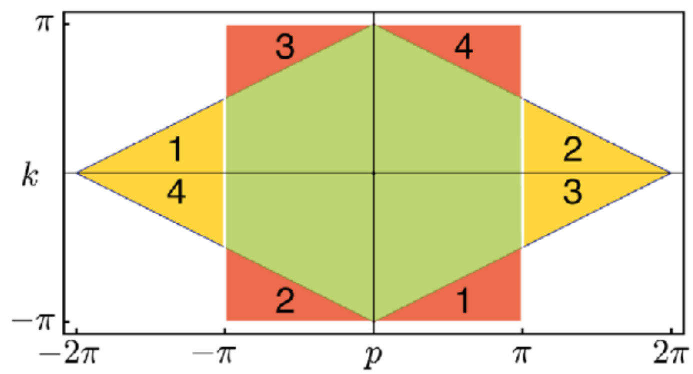


Figure 5.2.1: Rearrangement of the first Brillouin zone for variables (k,p) (see Eq. (5.2.4)) to run through $[-\pi,\pi]^2$.

Next, we write the wavefunctions in relative and total momentum. From (5.2.5) and (5.2.6), we deduce that

$$\hat{\psi}(k,p) = \sum_{d} \sum_{s\equiv d \bmod 2} e^{-\mathrm{i}sp/2} e^{-\mathrm{i}kd} \psi(s,d), \tag{5.2.7}$$

with inverse

$$\psi(s,d) = \frac{1}{(2\pi)^2} \int_{\mathbb{T}^2} e^{\mathrm{i}sp/2} e^{\mathrm{i}kd} \hat{\psi}(k,p)\, \mathrm{d}k\, \mathrm{d}p. \tag{5.2.8}$$

5.2.2 Fourier transformation of the IQW

Now, we perform the transformation of the interaction operator. Recall that given an operator $A \in \mathcal{L}(\mathcal{H}_2)$, its Fourier transform $\hat{A} \in \mathcal{L}(\hat{\mathcal{H}}_2)$ is such that $\hat{A} = \mathcal{F} A \mathcal{F}^{-1}$. Since $\mathcal{F}$ is a unitary transformation, A and $\hat{A}$ are said to be *unitarily equivalent* and have the same spectrum.

5.2.2.1 Transformation of $\mathcal{V}$

The interaction at position (x_1,x_2),

$$V(x_1,x_2) = \sum_{\sigma_1',\sigma_2'} \sum_{\sigma_1,\sigma_2} V_{\sigma_1\sigma_2}^{\sigma_1'\sigma_2'}(x_1,x_2) |\sigma_1'\sigma_2'\rangle\langle\sigma_1,\sigma_2|, \tag{5.2.9}$$

is an operator over the spin degrees of freedom, whose matrix elements are noted

$$\langle\sigma_1',\sigma_2'|\left(V(x_1,x_2)|\sigma_1,\sigma_2\rangle\right) = V_{\sigma_1\sigma_2}^{\sigma_1'\sigma_2'}(x_1,x_2). \tag{5.2.10}$$

[3]Thanks to A. Werner for allowing to reproduce this figure from [AAM+12].

Being $\mathcal{V}$ a multiplication operator in the direct space, in Fourier space it takes the form of a convolution, and furthermore with a kernel that only depends on the relative momentum. We now provide the details, assuming all along that hypothesis **(H0)** holds.

Since $\mathcal{V}$ is unitary, then $||V(x_1, x_2)||$ is a constant independent of position. Hence

$$\{V(x_1, x_2)\}_{x_1,x_2\in\mathbb{Z}} \in \mathcal{M}_4(\mathcal{S}'(\mathbb{Z}^2)), \tag{5.2.11}$$

i.e. it is a sequence of slow growth, and thus

$$\hat{V}(k_1, k_2) = \sum_{x_1,x_2} e^{-\mathrm{i}(k_1x_1+k_2x_2)}V(x_1, x_2) \tag{5.2.12}$$

converges to some $\hat{V} \in \mathcal{M}_4(\mathcal{P}'(\mathbb{R}^2))$, that is, to an object in the space of 4×4 matrices whose coefficients are periodic distributions of period 2π in two variables, over the complex field. Let us swap to the relative and total momentum variables $(k_1, k_2) \mapsto (k, p)$ via (5.2.4), noting that the sum in the right-hand side of (5.2.12) can be written in the variables sum and difference, $s = x_1 + x_2$ and $d = x_1 - x_2$, via (5.2.6). But since these variables preserve parity, the sum in s, d is restricted to $s \equiv d \mod 2$, and it is convenient to sum over the unrestricted integer variables a, d where $s = 2a + d$. Also recall that $V = V(d)$, since we assume that the interaction is radial. Thus,

$$\hat{V}(k, p) = \sum_d \sum_{s\equiv d \text{ mod } 2} e^{-\mathrm{i}(sp/2+kd)}V(d) \tag{5.2.13}$$

$$= \sum_d \left(\sum_a e^{-\mathrm{i}ap}\right) e^{-\mathrm{i}dp/2}e^{-\mathrm{i}kd}V(d) \tag{5.2.14}$$

$$= 2\pi \sum_d \delta(p)e^{-\mathrm{i}dp/2}e^{-\mathrm{i}kd}V(d), \tag{5.2.15}$$

where in the last equality we used the Poisson summation formula (cf. Example (C.1.1)), which reduces to a delta in the origin since we restrict to $p \in [-\pi, \pi]$.

Since $\mathcal{V}$ is a multiplication by the matrix V in the direct space, and since multiplication is Fourier transformed into convolution via property 5 of Theorem (C.2), we let $\hat{\mathcal{V}} \in \mathcal{L}(\hat{\mathcal{H}}_2)$ be defined as

$$(\hat{\mathcal{V}}\hat{\psi})(k, p) = (\hat{V} * \hat{\psi})(k, p). \tag{5.2.16}$$

Note that, as outlined in Remark C.1, by a density argument the property alluded to above extends to $L^2(\mathbb{T}^2)$ functions (in fact, the convolution integral makes sense more generally for any pair of $L^1(\mathbb{T}^2)$ functions).

Using (5.2.15), the right-hand side becomes

$$
\begin{aligned}
(\hat{\mathcal{V}}\hat{\psi})(k,p) &= \frac{1}{(2\pi)^2}\int_{\mathbb{T}}\mathrm{d}p'\int_{\mathbb{T}}\mathrm{d}k'\left[2\pi\sum_d \delta(p-p')e^{-\mathrm{i}d(p-p')/2}e^{-\mathrm{i}(k-k')d}V(d)\hat{\psi}(k',p')\right] \\
&= \frac{1}{2\pi}\int_{\mathbb{T}}\sum_d e^{-\mathrm{i}(k-k')d}\hat{\psi}(k',p)\mathrm{d}k' \\
&= \frac{1}{2\pi}\int_{\mathbb{T}}\hat{V}(k-k')\hat{\psi}(k',p)\mathrm{d}k'. \qquad (5.2.17)
\end{aligned}
$$

In the last equality we defined the “relative” Fourier transform of the interaction, that is,

$$
\hat{V}(k) = \sum_{x\in\mathbb{Z}} e^{-\mathrm{i}kx}V(x), \qquad \text{with inverse} \qquad V(x) = \frac{1}{2\pi}\int_{\mathbb{T}} e^{\mathrm{i}kx}\hat{V}(k)\mathrm{d}k, \qquad (5.2.18)
$$

where the series is convergent in $\mathcal{M}_4(\mathcal{P}'(\mathbb{R}))$.

It remains to check unitarity of $\hat{\mathcal{V}} \in \mathcal{L}(\hat{\mathcal{H}}_2)$. We can argue that since $\mathcal{V}$ is unitary, and since the Fourier map is a unitary operator, the claim follows. Alternatively we can directly compute in the reciprocal space, the adjoint operator of $\hat{\mathcal{V}}$ being defined by

$$
\langle\hat{\psi},\hat{\mathcal{V}}\hat{\varphi}\rangle = \langle\hat{\mathcal{V}}^\dagger\hat{\psi},\hat{\varphi}\rangle \qquad (5.2.19)
$$

for all pairs $\hat{\psi},\hat{\varphi}\in\hat{\mathcal{H}}_2$. Let us check that $\hat{\mathcal{V}}^\dagger$ is given by

$$
(\hat{\mathcal{V}}^\dagger\hat{\psi})(k) = (\tilde{\hat{V}} * \psi)(k) = \frac{1}{2\pi}\int_{\mathbb{T}}\hat{V}^\dagger(k'-k)\hat{\psi}(k')\mathrm{d}k' \qquad (5.2.20)
$$

(note the sign change in the argument of $\hat{V}$). Then

$$
\begin{aligned}
\langle\hat{\mathcal{V}}^\dagger\hat{\psi},\hat{\varphi}\rangle &= \frac{1}{2\pi}\int_{\mathbb{T}}\left[\frac{1}{2\pi}\int_{\mathbb{T}}\hat{V}^\dagger(k'-k)\hat{\psi}(k')\mathrm{d}k'\right]^\dagger\hat{\varphi}(k)\,\mathrm{d}k \\
&= \frac{1}{2\pi}\int_{\mathbb{T}}\hat{\psi}^\dagger(k')\left[\frac{1}{2\pi}\int_{\mathbb{T}}\hat{V}(k'-k)\hat{\varphi}(k)\mathrm{d}k\right]\mathrm{d}k' \\
&= \langle\hat{\psi},\hat{\mathcal{V}}\hat{\varphi}\rangle \qquad (5.2.21)
\end{aligned}
$$

as claimed. Then, unitarity follows from

$$\begin{aligned}(\mathcal{V}^\dagger\mathcal{V}\hat{\psi})(k) &= \frac{1}{(2\pi)^2}\int_{\mathbb{T}}\hat{V}^\dagger(k'-k)\left[\int_{\mathbb{T}}\hat{V}(k'-k'')\hat{\psi}(k'')\mathrm{d}k''\right]\mathrm{d}k' \\ &= \frac{1}{(2\pi)^2}\sum_{x'}V^\dagger(x')\int_{\mathbb{T}}e^{-\mathrm{i}(k'-k)x'}\left[\sum_{x}V(x)\int_{\mathbb{T}}e^{-\mathrm{i}(k'-k'')x}\hat{\psi}(k'')\mathrm{d}k''\right]\mathrm{d}k' \\ &= \frac{1}{(2\pi)^2}\sum_{x,x'}V^\dagger(x')V(x)e^{\mathrm{i}kx'}\int_{\mathbb{T}}e^{-\mathrm{i}(x+x')k'}\mathrm{d}k'\int_{\mathbb{T}}e^{\mathrm{i}k''x}\hat{\psi}(k'')\mathrm{d}k'' \\ &= \sum_x V^\dagger(-x)V(x)e^{-\mathrm{i}kx}\psi(x) \\ &= \sum_x I_4 e^{-\mathrm{i}kx}\psi(x) = \hat{\psi}(k). \end{aligned} \tag{5.2.22}$$

We have thus proved the following proposition.

Proposition 5.1. *The Fourier transform of $\mathcal{V}\in\mathcal{L}(\mathcal{H}_2)$ is $\hat{\mathcal{V}}\in\mathcal{L}(\hat{\mathcal{H}}_2)$, given by*

$$(\hat{\mathcal{V}}\hat{\psi})(k,p) = \frac{1}{2\pi}\int_{-\pi}^{\pi}\hat{V}(k-k')\hat{\psi}(k',p)\mathrm{d}k' \tag{5.2.23}$$

for all $\hat{\psi}\in\hat{\mathcal{H}}_2$, and where

$$\hat{V}(k) = \sum_{x\in\mathbb{Z}}e^{-\mathrm{i}kx}V(x), \tag{5.2.24}$$

and $V(x)\equiv V(x_1,x_2+x)$. The convergence of the series is understood in the sense of distributions, i.e. $\hat{V}(k)\in\mathcal{M}_4(\mathcal{P}'(\mathbb{R}))$. Moreover, the operator $\hat{\mathcal{V}}$ is unitary.

5.2.2.2 Transformation of $\mathcal{U}_0$ and $\mathcal{U}$

Next, we find the representation in Fourier space of the free and interacting walk operators.

Proposition 5.2. *For an IQW $\mathcal{U}=\mathcal{U}_0\mathcal{V}$, with $\mathcal{V}$ satisfying Assumptions **(H0)**, the following assertions hold:-*

(i) The free walk operator in Fourier space is

$$(\hat{\mathcal{U}}_0\hat{\psi})(k,p) = \Big(\hat{S}(k,p)(C_1\otimes C_2)\Big)\hat{\psi}(k,p)\equiv\hat{U}_0(k,p)\hat{\psi}(k,p),\qquad \hat{\psi}\in\hat{\mathcal{H}}_2, \tag{5.2.25}$$

that is, a multiplication operator by the matrix $\hat{U}_0(k,p)\in\mathcal{M}_4(\mathbb{C})$ whose entries are analytic in the variables $(k,p)\in\mathbb{T}^2$. Moreover, ordering the basis of $\mathbb{C}^2$ as $\{|\sigma=1\rangle,|\sigma=-1\rangle\}$, the shift matrix in Fourier space is $\hat{S}(k,p)=\mathrm{diag}(e^{-\mathrm{i}p},e^{-2\mathrm{i}k},e^{2\mathrm{i}k},e^{\mathrm{i}p})$.

(ii) The interacting walk operator in Fourier space is the unitary operator $\hat{\mathcal{U}}=\hat{\mathcal{U}}_0\cdot(\hat{V}*)$. In matrix form,

$$(\hat{\mathcal{U}}\hat{\psi})(k,p) = \hat{U}_0(k,p)\,\frac{1}{2\pi}\int_{-\pi}^{\pi}\hat{V}(k-k')\hat{\psi}(k',p)\mathrm{d}k'. \tag{5.2.26}$$

Proof. (i) Since $S_1|x_1,\sigma_1\rangle = |x_1+\sigma_1,\sigma_1\rangle$, it acts on wavefunctions as τ_{σ_1}. Indeed,

$$\begin{aligned}(S_1\otimes I_{\mathcal{H}_1})\psi &= \sum_{x_1,x_2,\sigma_2} \psi^{+\sigma_2}(x_1,x_2)|x_1+1,x_2,+,\sigma_2\rangle + \psi^{-\sigma_2}(x_1,x_2)|x_1-1,x_2,-,\sigma_2\rangle \\ &= \sum_{x_1,x_2,\sigma_2} \psi^{+\sigma_2}(x_1-1,x_2)|x_1,x_2,+,\sigma_2\rangle + \psi^{-\sigma_2}(x_1+1,x_2)|x_1,x_2,-,\sigma_2\rangle \\ &= \sum_{x_1,x_2,\sigma_2} (\tau_{1,0}\psi^{+\sigma_2}(x_1,x_2))|x_1,x_2,+,\sigma_2\rangle + (\tau_{-1,0}\psi^{-\sigma_2}(x_1,x_2))|x_1,x_2,-,\sigma_2\rangle,\end{aligned}$$

and consequently, using the translation property of the Fourier map (see part 1 of Theorem C.1), it is represented in Fourier space as

$$(\tau_{\sigma_1,0}\psi^{\sigma_1\sigma_2}(x_1,x_2))^\wedge(k_1,k_2) = e^{-\mathrm{i}\sigma_1 k_1}\hat{\psi}^{\sigma_1\sigma_2}(k_1,k_2). \tag{5.2.27}$$

The reasoning is analogous for S_2. Thus, we arrive at

$$\begin{aligned}\hat{S}_1\otimes\hat{S}_2 : \hat{\psi}(k_1,k_2) \to &\left[\begin{pmatrix} e^{-\mathrm{i}k_1} & 0 \\ 0 & e^{\mathrm{i}k_1}\end{pmatrix} \otimes \begin{pmatrix} e^{-\mathrm{i}k_2} & 0 \\ 0 & e^{\mathrm{i}k_2}\end{pmatrix}\right]\hat{\psi}(k_1,k_2) = \\ &= \begin{pmatrix} e^{-\mathrm{i}(k_1+k_2)} & & & \\ & e^{-\mathrm{i}(k_1-k_2)} & & \\ & & e^{\mathrm{i}(k_1-k_2)} & \\ & & & e^{\mathrm{i}(k_1+k_2)}\end{pmatrix}\hat{\psi}(k_1,k_2),\end{aligned}$$

which allows to conclude, using that $p = k_1+k_2$ and $2k = k_1-k_2$. Finally, the analyticity of matrix entries follows from the map $k \mapsto e^{\mathrm{i}k}$ being analytic.

(ii) The representation of $\mathcal{U}$ in Fourier space, Eq. (5.2.26), is obtained by combination of Proposition 5.1 and part (i) above. Moreover, it is unitary because it is the product of two unitary operators. □

To conclude the section, we give a simple consequence of $\mathcal{U}$ being translation invariant: that the total momentum p is a conserved quantity during the evolution. This is important because it allows to study the problem in the Hilbert space associated with a fixed value of momentum, that we call $\mathcal{H}_{2,p} \simeq \ell^2(\mathbb{Z})\otimes\mathbb{C}^4$, and the associated reciprocal space is denoted $\hat{\mathcal{H}}_{2,p} \simeq L^2(\mathbb{T})\otimes\mathbb{C}^4$. Hence, $\hat{\mathcal{U}}$ over $\hat{\mathcal{H}}_{2,p}$ is defined exactly as in (5.2.26) but where p is considered as a parameter and not as a variable.

Proposition 5.3. *Assuming **(H0)**,*

(i) $\mathcal{U}$ commutes with joint translations, and

(ii) the total momentum is preserved under the unitary evolution, i.e. in the semigroup $\{\mathcal{U}^t\psi_0 : t\in\mathbb{N}_0\}$ for each initial condition $\psi_0\in\mathcal{H}_2$.

Proof. (i) It suffices to develop the action of $\mathcal{U} = \mathcal{U}_0\mathcal{V}$ over an arbitrary basis ket of $\mathcal{H}_2$, and then use the definition of translation invariance. Recall that $\mathcal{U}$ is translation invariant if it commutes with $\tau_{x_0,x_0}\in\mathcal{L}(\mathcal{H}_2)$, defined as

$$\tau_{x_0,x_0}|x_1,x_2,\sigma_1,\sigma_2\rangle = |x_1+x_0,x_2+x_0,\sigma_1,\sigma_2\rangle, \qquad x_0\in\mathbb{Z}. \tag{5.2.28}$$

Indeed,

$$\begin{aligned}\mathcal{U}_0\mathcal{V}|x_1,x_2,\sigma_1,\sigma_2\rangle &= \mathcal{U}_0 V(x_1,x_2)|x_1,x_2\rangle|\sigma_1,\sigma_2\rangle \\ &= (S_1\otimes S_2)\cdot(I_{\mathbb{Z}^2}\cdot(C_1\otimes C_2))|x_1,x_2\rangle\sum_{\sigma_1'\sigma_2'} V_{\sigma_1\sigma_2}^{\sigma_1'\sigma_2'}(x_1,x_2)|\sigma_1',\sigma_2'\rangle \\ &= (S_1\otimes S_2)|x_1,x_2\rangle\sum_{\sigma_1'\sigma_2'} V_{\sigma_1\sigma_2}^{\sigma_1'\sigma_2'}(x_1,x_2)\sum_{\sigma_1''} C_{1\ \sigma_1'}^{\sigma_1''}|\sigma_1''\rangle\sum_{\sigma_2''} C_{2\ \sigma_2'}^{\sigma_2''}|\sigma_2''\rangle \\ &= \sum_{\sigma_1''\sigma_2''}\sum_{\sigma_1'\sigma_2'} C_{1\ \sigma_1'}^{\sigma_1''} C_{2\ \sigma_2'}^{\sigma_2''} V_{\sigma_1\sigma_2}^{\sigma_1'\sigma_2'}(x_1,x_2)|x_1+\sigma_1'',x_2+\sigma_2'',\sigma_1'',\sigma_2''\rangle.\end{aligned} \tag{5.2.29}$$

Using **(H0)**, $V(x_1,x_2)$ is assumed to be radial hence depending only on $|x_1-x_2|$, and from this fact one easily checks that $[\tau_{x_0,x_0},\mathcal{U}]=0$ for any $x_0\in\mathbb{Z}$ over an arbitrary basis ket.

(ii) It is an elementary fact from quantum mechanics that the momentum is the generator of translations, so part (i) above allows to conclude. More directly, one sees that Eq. (5.2.26) in Proposition 5.2 only acts on the p coordinate via multiplication with the unitary matrix $\hat{U}_0(k,p)$. □

5.3 Basic properties of the free QW

This section is advocated to the study of the spectral properties of the free walk operator. In particular we completely characterize the location of the spectral gaps of $\mathcal{U}_0$ in full generality, that is, for arbitrary choices of parameters.

We collect in Appendix C.2 the elements of spectral theory in Hilbert space that will be used in this and in the following sections.

5.3.1 Overview

Recall that $U(n)$ is n^2-parametric, therefore an arbitrary $C\in U(2)$ is parametrized by four real parameters. We choose the following parametrization:

$$C = e^{\mathrm{i}\theta}\begin{pmatrix} re^{-\mathrm{i}\alpha} & \mathrm{i}e^{\mathrm{i}\gamma}\sqrt{1-r^2} \\ \mathrm{i}e^{-\mathrm{i}\gamma}\sqrt{1-r^2} & re^{\mathrm{i}\alpha}\end{pmatrix}, \tag{5.3.1}$$

with $\alpha,\gamma,\theta\in[0,2\pi)$ and $r\in[0,1]$. These parameters reduce to three if the global factor $e^{\mathrm{i}\theta}$ is discarded ($\theta=0$). Usually this is the case in homogeneous QWs, because a global, constant, phase factor does not show up in the dynamics. However we shall not throw it away since we are interested in location of spectra, and it is in fact relevant to be able to rotate freely the location of the spectrum of the free QW, before we plug-in the interaction.

In this section we are interested in the spectrum of the free QW $\mathcal{U}_0$ in the relative coordinate, that is, for fixed p. We shall study the influence of each parameter r,α,γ,θ in the band structure. Moreover, we are interested in some special points which play a particular role in the spectral properties of the perturbed operator, these are called critical points $\mathcal{U}_0$-*critical points* in [ABJ15].

Definition 5.2. *(see [ABJ15]) Quasienergy values which correspond either to band crossings or to critical points (or both) are called* $\mathcal{U}_0$-critical points. *We denote this set by* $M_{\mathcal{U}_0} \subset \mathbb{T}$.

5.3.2 One-dimensional case

It is illustrative to understand the one-dimensional case first in order to see what is the role of each coin parameters on the spectrum.

Let C be given by Eq. (5.3.1), and let $\hat{S}(k) = \mathrm{diag}\{e^{-\mathrm{i}k}, e^{\mathrm{i}k}\}$. The spectrum of $\hat{S}(k)C$ as a set are the values of

$$\lambda_\pm(k) = e^{\mathrm{i}\theta} e^{\pm \mathrm{i}\omega(k)}, \qquad \text{where } \cos\omega(k) = r\cos(\alpha + k). \tag{5.3.2}$$

Note that the parameter γ does not appear. The parameter θ is just a global phase, i.e. a rotation. The role of the parameters r and α is best understood looking at the phase of $\lambda_\pm(k)$, whose variation depends on $\omega(k)$ as a function of $k \in \mathbb{T}$. Let us concentrate on $\lambda_+(k)$ first, and $\theta = 0$. Note that $\cos\omega(k)$ is a function onto $[-r, r]$, which is a symmetric interval around 0; hence the phase $\omega(k)$ is onto $[\arccos(-r), \arccos(r)]$, which is an interval centred around $\pi/2$. The boundary points give the edges of the bands, thus they are located at $e^{\mathrm{i}\arccos(-r)}$ and $e^{\mathrm{i}\arccos(r)}$. This analysis extends easily for λ_-, since for $\theta = 0$, it is just the complex conjugate of λ_+, hence symmetric to it with respect to the real axis. For $\theta \neq 0$, both λ_+ and λ_- are rotated by the same factor θ, in the positive direction (counterclockwise) for positive θ and in the negative direction for negative θ.

We conclude that there are two bands,

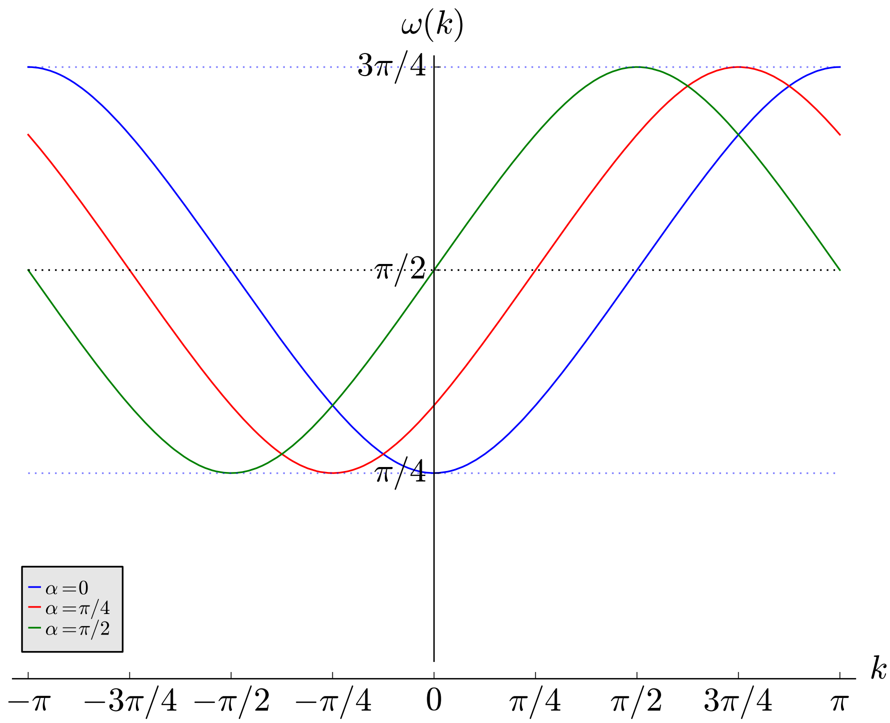
$$\begin{aligned} B_+ &= e^{\mathrm{i}\theta}[\mu_+, \mu'_+], \text{ with } \mu_+ = r + \mathrm{i}\sqrt{1-r^2},\ \mu'_+ = -r + \mathrm{i}\sqrt{1-r^2}, && (5.3.3)\\ B_- &= e^{\mathrm{i}\theta}[\mu_-, \mu'_-], \text{ with } \mu_- = -r - \mathrm{i}\sqrt{1-r^2},\ \mu'_- = r - \mathrm{i}\sqrt{1-r^2}, && (5.3.4)\\ & \text{and } |B_+| = |B_-| = 2\arcsin r. && (5.3.5) \end{aligned}$$

Hence r controls the arc length of the bands, since $|B_\pm|$ is a monotonically increasing function of r, from a point, i.e. $|B_\pm| = 0$ for $r = 0$, to a whole semi-circle, i.e. $|B_\pm| = \pi$ for $r = 1$. The role of α is to control for which values of k the extremal points of the bands are reached. Hence it does not show up in the spectrum of $\mathbb{T}$, but just shifts the phase $\omega(k)$. These observations are shown in Figures 5.3.1 and 5.3.2.

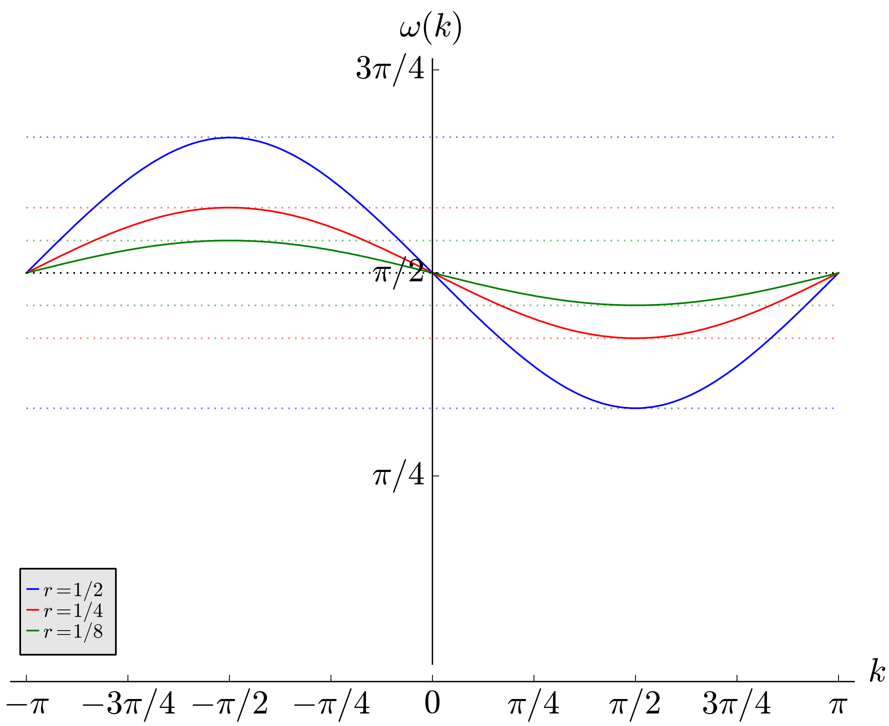
5.3.2.1 Critical points

Critical points are obtained computing

$$\nabla_k \lambda_\pm(k) = 0 \iff \alpha + k = n\pi, n \in \mathbb{Z}. \tag{5.3.6}$$

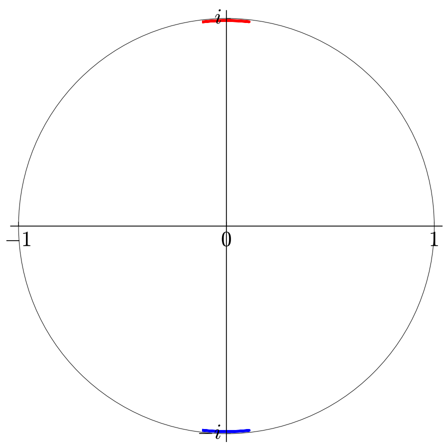


(a) $r = 1/\sqrt{2}$ and $\alpha = 0, \pi/4, \pi/2$.

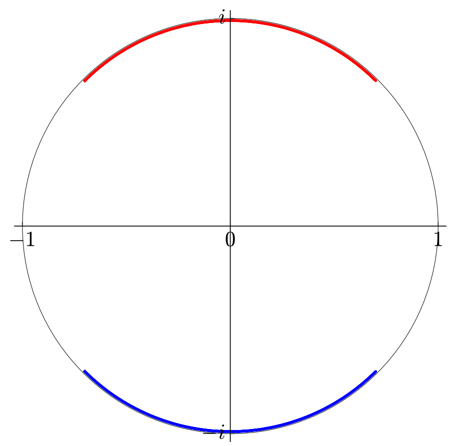


(b) $r = 1/2, 1/4, 1/8$, and $\alpha = 3\pi/2$.

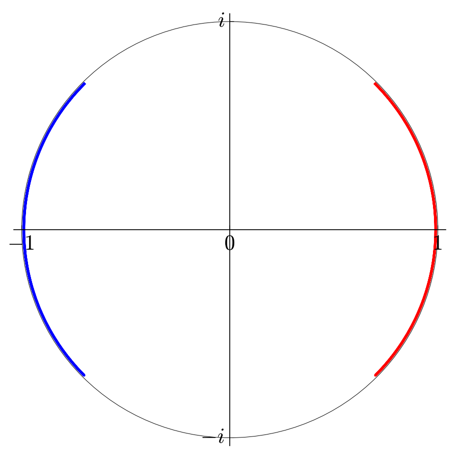
Figure 5.3.1: Graph of $\omega(k)$, for different values of the parameters r, α. The parameter α controls the relative shift of $\omega(k)$, while the parameter r controls its amplitude.



(a) $\theta = 0$, $r = 1/9$.



(b) $\theta = 0$, $r = 1/\sqrt{2}$



(c) $\theta = 3\pi/2$, $r = 1/\sqrt{2}$

Figure 5.3.2: Spectrum of the free walk operator in the one-dimensional case. In red (resp. blue) the band B_+ (resp B_-). The parameter r controls the arc length of the bands, and θ performs a rotation in the positive direction.

Indeed, the relative extrema are given by

$$\frac{d\omega}{dk} = 0 \iff \frac{r\sin(\alpha + k)}{\sqrt{1 - r^2\cos(\alpha + k)^2}} = 0 \iff \alpha + k = n\pi, n \in \mathbb{Z}. \tag{5.3.7}$$

Since $k \in \mathbb{T}$, $\alpha \in [0, 2\pi)$, there are at least two relative extrema of $\omega(k)$ (three in the special cases $\alpha = 0, \pi$ but they appear at the boundary points of k). Evaluating $\lambda_\pm(k)$ at these points, we obtain the edges of the bands.

5.3.2.2 Band crossings

Band crossings are obtained computing

$$\lambda_+(k) = \lambda_-(k) \iff \omega(k) = -\omega(k) + 2n\pi, n \in \mathbb{Z}. \tag{5.3.8}$$

Hence $\omega(k) = n\pi, n \in \mathbb{Z}$, implying $r\cos(\alpha + k) = \pm 1$, which holds provided that $r = 1, \alpha + k = n\pi, n \in \mathbb{Z}$. In particular, they are only possible if $r = 1$, observation which is clear from the graphs.

5.3.2.3 Summary

We have thus proved the following statement, cf. [ABJ15], Prop. 4.1.

Proposition 5.4. *For the one-dimensional case, the $\mathcal{U}_0$-critical points are*

$$M_{\mathcal{U}_0} = \left\{ e^{\mathrm{i}\theta}(-r \pm \mathrm{i}\sqrt{1-r^2}), e^{\mathrm{i}\theta}(r \pm \mathrm{i}\sqrt{1-r^2}) \right\}. \tag{5.3.9}$$

Remark 5.2. From a physical point of view we can interpret the results by looking at the dependence of the band arc length on r. We obtained that for $r \in (0, 1]$ there is only continuous spectrum, hence we have propagation. Indeed for $r \simeq 1$, C is close to the identity, in the sense that the weight of its coefficients is dominated by the diagonal terms, and the continuous spectrum covers the full circle. Now, a QW with a coin close to the identity favours propagation in both directions, the limiting case being $C = I_2$ for $r = 1$, in which case there is no coin mixture at all, i.e. any state $|x\rangle|\pm 1\rangle$, $x \in \mathbb{Z}$, just propagates to the right, resp. left.

Conversely, for $r \simeq 0$, C is close to the Pauli matrix σ_x, in the sense that the weight of its coefficients is dominated by the anti-diagonal terms. In the limiting case we have $C = \sigma_x$ for $r = 0$, and there is only point spectrum. Indeed since σ_x just flips the coin state at each time step, it does not allow for propagation, as the following simple calculation shows. Consider an initial state $|\psi_0\rangle = |x\rangle|1\rangle$, $x \in \mathbb{Z}$, then

$$|x\rangle|1\rangle \overset{I_{\mathbb{Z}}\otimes C}{\to} |x\rangle|-1\rangle \overset{S}{\to} |x-1\rangle|-1\rangle \overset{I_{\mathbb{Z}}\otimes C}{\to} |x-1\rangle|1\rangle \overset{S}{\to} |x\rangle|1\rangle \overset{I_{\mathbb{Z}}\otimes C}{\to} \dots$$

5.3.2.4 Eigenvectors

The eigenvectors of $\hat{S}(k)C$, with $C = C(\theta, r, \alpha, \gamma)$ (see Eq. (5.3.1)) are computed below. Recall that the eigenvalues are $\lambda_\pm(k) = e^{\mathrm{i}\theta}e^{\pm\mathrm{i}\omega(k)}$, $\cos\omega(k) = r\cos(\alpha + k)$. The normalized eigenvectors are

$$|u_\pm\rangle = \frac{1}{\sqrt{2N_\pm(k)}} \left(e^{\mathrm{i}(\gamma - k)}, \frac{\pm\sin\omega(k) + r\sin(\alpha + k)}{\sqrt{1-r^2}} \right)^{\mathrm{T}}, \tag{5.3.10}$$

and the normalization constant is

$$N_{\pm}(k) = \frac{1}{2}\left(1 + \frac{(\pm\sin\omega(k) + r\sin(\alpha+k))^2}{1-r^2}\right) \tag{5.3.11}$$

$$= \frac{\sin\omega(k)}{1-r^2}\left(\sin\omega(k) \pm r\sin(\alpha+k)\right). \tag{5.3.12}$$

Example 5.3.1. A particular instance of (5.3.1) is the Hadamard coin. It has been widely used in the context of QWs because under a suitable initial condition it leads to symmetric probability distribution functions. The analysis in Fourier space of the Hadamard QW is often used to obtain the explicit analytic solutions and it can be found in many places; a complete treatment is found for instance in pp. 70-73 of [Por13]. The Hadamard coin is obtained letting $\alpha = \theta = 3\pi/2$, $\gamma = 0$, $r = 1/\sqrt{2}$, which gives

$$C = \frac{1}{\sqrt{2}}\begin{pmatrix} 1 & 1 \\ 1 & -1 \end{pmatrix}. \tag{5.3.13}$$

In this case, $\cos\omega(k) = \dfrac{\sin k}{\sqrt{2}}$. Using the previous formulas and straightforward simplifications we compute below the eigenvalues and normalized eigenvectors of the associated free QW. The eigenvalues are explicitly

$$\lambda_{\pm}(k) = e^{\mathrm{i}(3\pi/2 \pm \arccos(\sin k/\sqrt{2}))} = \frac{\pm\sqrt{1+\cos^2 k} - \mathrm{i}\sin k}{\sqrt{2}}. \tag{5.3.14}$$

Its normalized eigenvectors are

$$|u_{\pm}\rangle = \frac{1}{\sqrt{2N_{\pm}(k)}}\left(e^{-\mathrm{i}k}, \pm\sqrt{1+\cos^2 k} - \cos k\right)^{\mathrm{T}}, \tag{5.3.15}$$

and the normalization constant is

$$N_{\pm}(k) = 1 + \cos^2 k \pm \cos k\sqrt{1+\cos^2 k}. \tag{5.3.16}$$

5.3.3 Two-dimensional case

Let $C_j = C_j(\theta_j, r_j, \alpha_j, \gamma_j)$, $j = 1, 2$, being

$$C_j = e^{\mathrm{i}\theta_j}\begin{pmatrix} r_j e^{-\mathrm{i}\alpha_j} & \mathrm{i}e^{\mathrm{i}\gamma_j}\sqrt{1-r_j^2} \\ \mathrm{i}e^{-\mathrm{i}\gamma_j}\sqrt{1-r_j^2} & r_j e^{\mathrm{i}\alpha_j} \end{pmatrix}, \tag{5.3.17}$$

where $\alpha_j, \gamma_j, \theta_j \in [0, 2\pi)$ and $r_j \in [0, 1]$. Without loss of generality we set $\theta_2 = \theta - \theta_1$. The spectrum of $\hat{U}_0$ is obtained combining (5.2.25) with relations (5.2.5),

$$\begin{aligned}\sigma(\hat{U}_0) = \sigma\left[(\hat{S}_1 \otimes \hat{S}_2) \cdot (C \otimes C)\right] &= \sigma\left[\hat{S}_1 C_1 \otimes \hat{S}_2 C_2)\right] \\ &= \sigma(\hat{S}_1 C_1)\sigma(\hat{S}_2 C_2) \\ &= e^{\mathrm{i}\theta_1} e^{\mathrm{i}\theta_2} \left\{e^{\mathrm{i}(\omega_1+\omega_2)}, e^{-\mathrm{i}(\omega_1+\omega_2)}, e^{\mathrm{i}(\omega_1-\omega_2)}, e^{-\mathrm{i}(\omega_1-\omega_2)}\right\} \\ &= \{\lambda_{1,+}, \lambda_{1,-}, \lambda_{2,+}, \lambda_{2,-}\},\end{aligned}$$

where

$$\lambda_{1,\pm} = e^{\mathrm{i}\theta} e^{\pm \mathrm{i}(\omega_1+\omega_2)}, \qquad \lambda_{2,\pm} = e^{\mathrm{i}\theta} e^{\pm \mathrm{i}(\omega_1-\omega_2)}, \tag{5.3.18}$$

and

$$\cos\omega_1 = r_1 \cos(\alpha_1 + p/2 + k) \text{ and } \cos\omega_2 = r_2 \cos(\alpha_2 + p/2 - k). \tag{5.3.19}$$

First note that the parameter θ is just a global phase, i.e. a rotation. The general disposition of the bands over the unit circle, for a fixed choice of parameters and fixed value of total momentum p, is best understood looking at the properties of the phase functions of $\lambda_{1,\pm}$ and $\lambda_{2,\pm}$, namely $\pm(\omega_1(k)+\omega_2(k))$ and $\pm(\omega_1(k)-\omega_2(k))$, respectively, as a function of $k \in \mathbb{T}$. We assert the key properties as a lemma.

Lemma 5.1. *The phase functions $\omega_1(k) + \omega_2(k)$ and $\omega_1(k) - \omega_2(k)$, $k \in \mathbb{T}$, satisfy the following properties:*

(i) If $\varphi_1 \in \mathrm{Im}(\omega_1 + \omega_2)$, then $2\pi - \varphi_1 \in \mathrm{Im}(\omega_1 + \omega_2)$.

(ii) If $\varphi_2 \in \mathrm{Im}(\omega_1 - \omega_2)$, then $-\varphi_2 \in \mathrm{Im}(\omega_1 - \omega_2)$.

(iii) $\pi \in \mathrm{Im}\,(\omega_1 + \omega_2)$.

(iv) $0 \in \mathrm{Im}\,(\omega_1 - \omega_2)$.

Proof. For (i) and (ii), note that

$$\begin{aligned}\omega_1(k) = \arccos(r_1\cos(\alpha_1 + p/2 + k)) \Rightarrow \omega_1(k \pm \pi) = \arccos(-r_1\cos(\alpha_1 + p/2 + k)), \\ \omega_2(k) = \arccos(r_2\cos(\alpha_2 + p/2 - k)) \Rightarrow \omega_2(k \pm \pi) = \arccos(-r_2\cos(\alpha_2 + p/2 - k)),\end{aligned}$$

and recall the identity $\arccos(x) + \arccos(-x) = \pi$, $x \in [-1, 1]$. It is clear that given $k \in [-\pi, \pi]$, we can always find either $k + \pi$ or $k - \pi$ to be in $[-\pi, \pi]$ (or both, in the special case $k = 0$, in which $k = \pi$ and $k = -\pi$ are identified). Now if $\varphi_1 \in \mathrm{Im}(\omega_1 + \omega_2)$, then

$$\varphi_1 = \omega_1(k) + \omega_2(k) = \pi - \omega_1(k \pm \pi) + \pi - \omega_2(k \pm \pi)$$

implies that

$$2\pi - \varphi_1 \in \mathrm{Im}(\omega_1 + \omega_2).$$

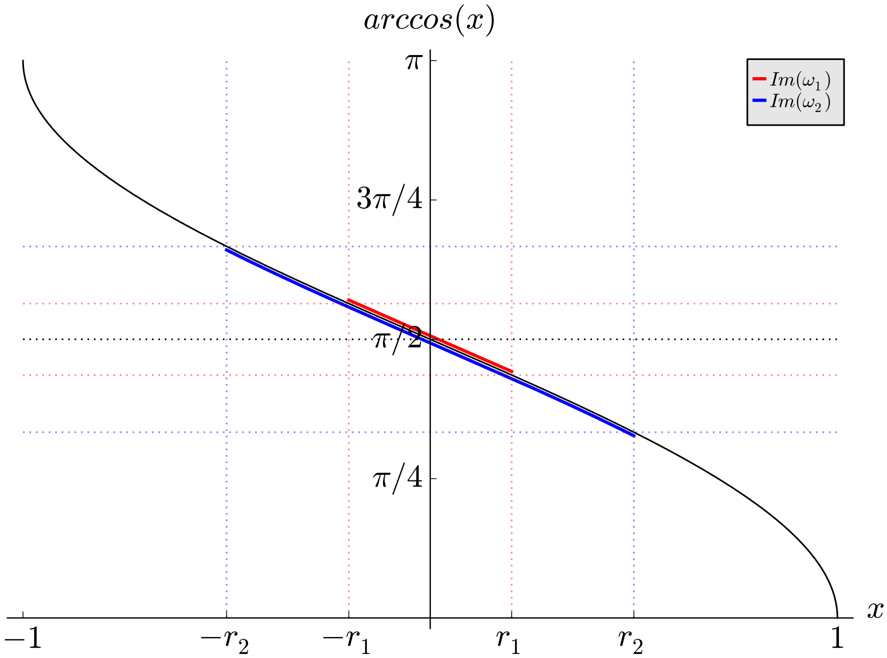


Figure 5.3.3: Plot of the arccosine function and its restriction to the symmetric intervals $-r_1 \leq x \leq r_1$ and $-r_2 \leq x \leq r_2$; the projection of the coloured segments on the vertical axis being the image set of ω_1 and ω_2 respectively.

In a similar way, if $\varphi_2 \in \mathrm{Im}(\omega_1 - \omega_2)$, then

$$\varphi_2 = \omega_1(k) - \omega_2(k) = \pi - \omega_1(k \pm \pi) - \pi + \omega_2(k \pm \pi)$$

implies that

$$-\varphi_2 \in \mathrm{Im}(\omega_1 - \omega_2).$$

For (iii) and (iv), first we remark that the images of $\omega_1(k)$ and $\omega_2(k)$ are

$$\mathrm{Im}\,\omega_1 = [\arccos(-r_1), \arccos(r_1)] \subseteq [0, \pi],$$

and

$$\mathrm{Im}\,\omega_2 = [\arccos(-r_2), \arccos(r_2)] \subseteq [0, \pi]$$

(see Fig. 5.3.4 for an example). Then, since $\omega_1(k)$ and $\omega_2(k)$ are continuous functions of $k \in \mathbb{T}$, part (i) (resp. part (ii)) implies that the point π must be crossed by $\omega_1(k) + \omega_2(k)$ (resp. the point 0 must be crossed by $\omega_1(k) - \omega_2(k)$). $\square$

Let $B_{1,\pm}$ (resp. $B_{2,\pm}$) be the bands associated with $\lambda_{1,\pm}$ (resp. $\lambda_{2,\pm}$). Assume for a moment that $\theta = 0$. The content of Lemma 5.1 is that $B_{1,+}$ (resp. $B_{2,+}$) is symmetric with respect to the real axis and the point $-1 \in B_{1,+}$ (resp. the point $1 \in B_{2,+}$). Moreover, $B_{1,-}$ (resp. $B_{2,-}$) is the complex conjugate of $B_{1,+}$ (resp. $B_{2,+}$), hence is obtained symmetrizing with respect to the real axis. With this information we conclude that there will be two pairs of bands, with $B_{1,+} = B_{1,-}$ and $B_{2,+} = B_{2,-}$ (of course the band crossings only happen

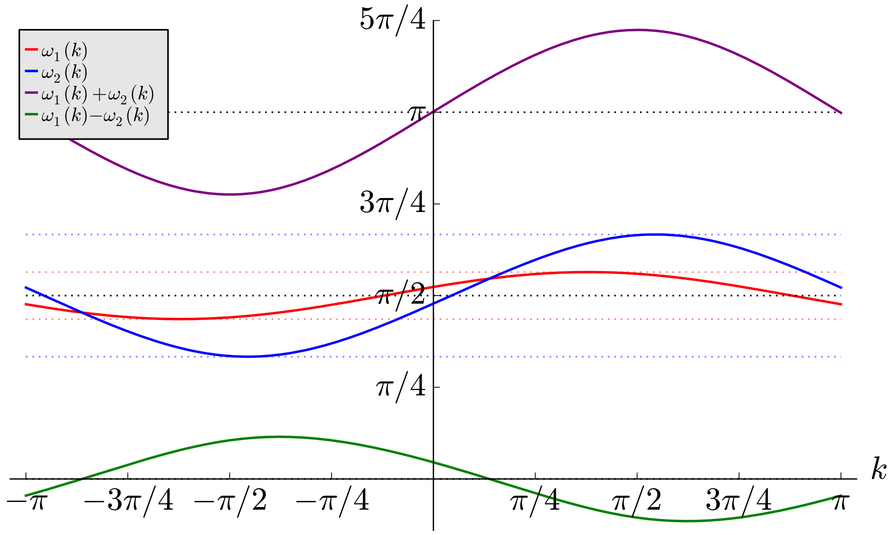


Figure 5.3.4: Typical behaviour of the phase functions $\omega_1(k)$, $\omega_2(k)$, their sum and their difference. A numerical evaluation shows that $\omega_1(k) + \omega_2(k) = \pi$ at $k = -0.0079, 3.13$, while $\omega_1(k) - \omega_2(k) = 0$ at $k = -2.71, 0.43$. Here we have chosen $r_1 = 0.2$, $r_2 = 0.5$, $\alpha_1 = 0.7$, $\alpha_2 = 3.6$, $\theta = 0$, and $p = 2.5$. The corresponding bands in the unit circle are shown in Fig. 5.3.5.(a).

when they coincide in the same value of k, which is a different thing). Finally note that if $\theta > 0$, the previous analysis still holds, although all the bands have to be rotated by θ in the positive (counter-clockwise) direction. Consequently, we arrive at

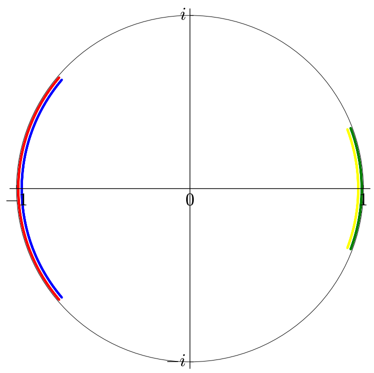
$$B_{1,+} = B_{1,-} = \mathrm{Im}\,(\lambda_{1,+}) = \mathrm{Im}\,(\lambda_{1,-}), \tag{5.3.20a}$$
$$B_{2,+} = B_{2,-} = \mathrm{Im}\,(\lambda_{2,+}) = \mathrm{Im}\,(\lambda_{2,-}). \tag{5.3.20b}$$

The bands will be noted

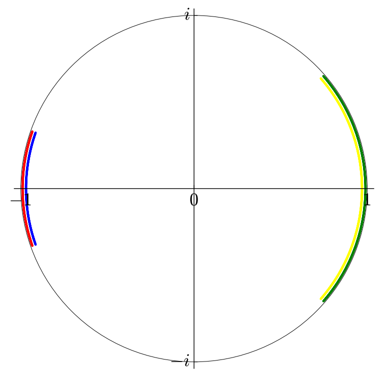
$$B_{1,+} := [\mu_1, \mu_1'] \subset \mathbb{S}, \tag{5.3.21a}$$
$$B_{2,+} := [\mu_2, \mu_2'] \subset \mathbb{S}. \tag{5.3.21b}$$

We show some plots of the spectrum in Fig. 5.3.5.

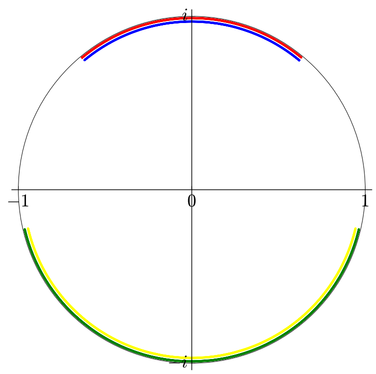
Remark 5.3. In contrast to the one-dimensional case, in the two-dimensional case the role of the radial parameters r_1, r_2 and of the angular parameters α_1, α_2 is not decoupled. For instance, in the one-dimensional case we saw that the arc lengths and the position of the edges of the bands on the unit circle depended only on r (and not on α, cf. Eqs. (5.3.3)-(5.3.5)), and conversely, the position of the relative extrema (corresponding to the band edges) depended only on α (cf. Eq. (5.3.7)). However both radial and angular parameters intervene, in general, in the two-dimensional setting. Intuitively this can be understood noting that the arc obtained from the product $e^{\mathrm{i}\omega_1(k)}e^{\mathrm{i}\omega_2(k)}$, will not depend on each factor individually but rather on the link imposed by k. More precisely, the return points, which are obtained optimizing $\omega_1(k) \pm \omega_2(k)$, depend in general on all the parameters. As an



(a) $r_1 = 0.2$, $r_2 = 0.5$, $\alpha_1 = 0.7$, $\alpha_2 = 3.6$, $\theta = 0$, and $p = 2.5$.



(b) $r_1 = 0.2$, $r_2 = 0.5$, $\alpha_1 = 0.7$, $\alpha_2 = 3.6$, $\theta = 0$, and $p = -1.5$.



(c) $r_1 = r_2 = 1/\sqrt{2}$, $\alpha_1 = \alpha_2 = 3\pi/2$, $\theta = 3\pi/2$, and $p = 1$.

Figure 5.3.5: Spectrum of $\mathcal{U}_0$. In red (resp. blue) are plotted the bands $B_{1,+}$ (resp $B_{1,-}$). In green (resp. yellow) are plotted the bands $B_{2,+}$ (resp $B_{2,-}$). Plots (a) and (b) differ just in the total momentum, which influences the respective arc lengths. In plot (c) the spectrum is rotated, $\theta \neq 0$.

illustration of this point, as we will see, for the choice in which the two individual arcs are of the same length, i.e. $r_1 = r_2 = r$, the position of the relative maxima of $\omega_1(k) \pm \omega_2(k)$ do not longer depend on r.

Next, we move on to calculate the $\mathcal{U}_0$-critical points. In the process we will find explicit formulas for the localization of the bands for arbitrary choices of parameters.

5.3.3.1 Critical points

We need to solve for k in

$$\frac{d}{dk}(\omega_1(k) + s\omega_2(k)) = 0, \tag{5.3.22}$$

with $k \in \mathbb{T}$, and where $s = \pm 1$. We shall introduce some notation. Let $\tilde{r}_1$, $\tilde{r}_2$ in $[0, \pi/2]$ such that $r_1 = \cos \tilde{r}_1$ and $r_2 = \cos \tilde{r}_2$; they exist and are unique because r_1 and r_2 are in $[0, 1]$. Also let $\tilde{\alpha}_1 = 2\alpha_1 + p \mod 2\pi$ and $\tilde{\alpha}_2 = 2\alpha_2 + p \mod 2\pi$.

Lemma 5.2. *Solutions of Eq.* (5.3.22) *reduce to those of*

$$c = a \cos 2k + b \sin 2k, \tag{5.3.23}$$

and where a, b, c do not depend on k and are given by

$$\begin{aligned} a &= \cos^2 \tilde{r}_1 \sin^2 \tilde{r}_2 \cos \tilde{\alpha}_1 - \sin^2 \tilde{r}_1 \cos^2 \tilde{r}_2 \cos \tilde{\alpha}_2, && (5.3.24a) \\ b &= -\cos^2 \tilde{r}_1 \sin^2 \tilde{r}_2 \sin \tilde{\alpha}_1 - \sin^2 \tilde{r}_1 \cos^2 \tilde{r}_2 \sin \tilde{\alpha}_2, && (5.3.24b) \\ c &= \cos^2 \tilde{r}_1 - \cos^2 \tilde{r}_2. && (5.3.24c) \end{aligned}$$

Moreover, the inequality

$$\Delta \equiv a^2 + b^2 - c^2 \geq 0 \tag{5.3.25}$$

holds for all possible choices of parameters.

Proof. Computing the derivative of the arccosine functions to each term separately (see Eq. (5.3.19)), we get

$$\frac{r_1 \sin(\alpha_1 + p/2 + k)}{\sqrt{1 - r_1^2 \cos^2(\alpha_1 + p/2 + k)}} - s \frac{r_2 \sin(\alpha_2 + p/2 - k)}{\sqrt{1 - r_2^2 \cos^2(\alpha_2 + p/2 - k)}} = 0. \tag{5.3.26}$$

Let $A = \tilde{\alpha}_1/2 + k$, $B = \tilde{\alpha}_1/2 - k$, square (5.3.26) and rearrange, obtaining

$$r_1^2 \sin^2 A - r_2^2 \sin^2 B = r_1^2 r_2^2 \sin^2 A \cos^2 B - r_1^2 r_2^2 \cos^2 A \sin^2 B. \tag{5.3.27}$$

Multiplying by 2 and using the identity $2 \sin^2 x = 1 - \cos 2x$ in the left-hand side, and factoring the right-hand side, we get

$$\begin{aligned} r_1^2(1 - \cos 2A) - r_2^2(1 - \cos 2B) &= 2r_1^2 r_2^2 (\sin A \cos B - \cos A \sin B)(\sin A \cos B + \cos A \sin B) \\ &= 2r_1^2 r_2^2 \sin(A + B) \sin(A - B). && (5.3.28) \end{aligned}$$

To conclude we shall invert the change of variables. Note that

$$\begin{aligned} \cos 2A &= \cos(2A - 2k + 2k) = \cos \tilde{\alpha}_1 \cos 2k - \sin \tilde{\alpha}_1 \sin 2k \\ \cos 2B &= \cos(2B + 2k - 2k) = \cos \tilde{\alpha}_2 \cos 2k + \sin \tilde{\alpha}_2 \sin 2k \\ 2 \sin(A + B) \sin(A - B) &= [\cos \tilde{\alpha}_2 - \cos \tilde{\alpha}_1] \cos 2k + [\sin \tilde{\alpha}_2 + \sin \tilde{\alpha}_1] \sin 2k. \end{aligned}$$

Substituting these expressions in Eq. (5.3.28) and rearranging, we get the final result

$$\underbrace{r_1^2 - r_2^2}_{c} = \cos 2k \left[\underbrace{r_1^2(1-r_2^2)\cos\tilde{\alpha}_1 - r_2^2(1-r_1^2)\cos\tilde{\alpha}_2}_{a} \right] + \sin 2k \left[\underbrace{-r_1^2(1-r_2^2)\sin\tilde{\alpha}_1 - r_2^2(1-r_1^2)\sin\tilde{\alpha}_2}_{b} \right].$$

Hence we obtain Eqs. (5.3.23)-(5.3.24c) by substituting $\cos\tilde{r}_1 = r_1$ and $\cos\tilde{r}_2 = r_2$.

To prove inequality (5.3.25), we set $\Delta = a^2+b^2-c^2$, and after a rather long factorization it turns out to be

$$\Delta = 4\cos^2\tilde{r}_1\cos^2\tilde{r}_2\sin^2\tilde{r}_1\sin^2\tilde{r}_2\sin^2(\tilde{\alpha}_1/2+\tilde{\alpha}_2/2), \tag{5.3.29}$$

which is non-negative. □

Remark 5.4. If $k^* \in [-\pi,\pi]$ is solution of $c = a\cos 2k + b\sin 2k$, then $k^* \pm \pi$ is a solution of the same equation, because

$$b\cos(2k^*) + c\sin(2k^*) = b\cos(2(k^*\pm\pi)) + c\sin(2(k^*\pm\pi)).$$

Moreover we can always choose $k^{**} \in [-\pi,\pi]$ such that $|k^{**}-k^*| = \pi$. We conclude that the different roots (for the same sign choice, because they are different branches of the tangent) are separated by π. Note that from Lemma 5.1 we knew that the return points for $\theta = 0$ had to be one the complex conjugate of the other, and obtained with a shift in π in the domain of k.

We move on to calculate the explicit solutions of Eq. (5.3.23). A convenient trick is to perform a Weierstrass substitution,

$$\cos 2k = \frac{1-u^2}{1+u^2},\ \sin 2k = \frac{2u}{1+u^2},\ \tan k = u, \qquad u\in\mathbb{R}, \tag{5.3.30}$$

which substituting in Eq. (5.3.23), gives

$$u^2(a+c) - 2bu - (a-c) = 0. \tag{5.3.31}$$

Solving for u,

$$u = \frac{b}{a+c} \pm \frac{\sqrt{\Delta}}{a+c}, \tag{5.3.32}$$

where $a+c \neq 0$ was assumed. The discriminant of (5.3.31) is thus proportional to Δ, which we know from inequality (5.3.25) of Lemma 5.2 that is non-negative. The possibilities for the roots are shown in the tree below.

if

- $a + c \neq 0$
  - $\Delta > 0$ — $k_1 \neq k_2$
  - $\Delta = 0$ — $k_1 = k_2$
- $a + c = 0$
  - $b = 0$
    - $a = c$ — $\forall k \in \mathbb{T}$
    - $a \neq c$ — $\emptyset$
  - $b \neq 0$ — $\tan k = \frac{c}{b}$ (1)

(1) If also $c = 0$, then the poles at $\pm\pi/2$ are also roots of (5.3.23).

In the following we assume the non-trivial cases $r_1, r_2 \in (0, 1)$. Let us introduce the quantity

$$R = \tan \tilde{r}_2 \cot \tilde{r}_1 = \sqrt{\frac{r_2^{-2} - 1}{r_1^{-2} - 1}}, \qquad r_1, r_2 \in (0, 1), \tag{5.3.33}$$

which is a continuous function on $(0, 1) \times (0, 1)$, and has divergent behaviour in the limits $r_1 \to 1$ and $r_2 \to 0$. The contour levels are shown in Fig. 5.3.6.

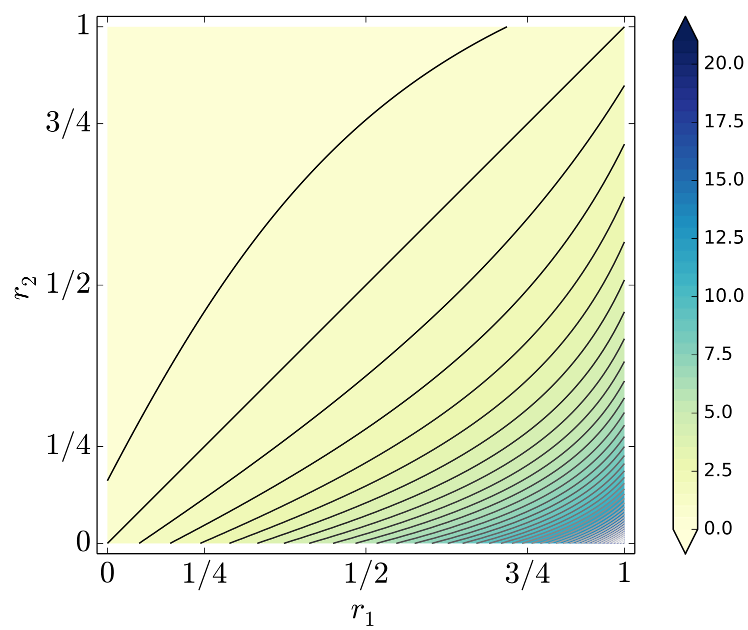


Figure 5.3.6: Contour levels of the function $R = R(r_1, r_2)$, and for plotting convenience we restricted to $r_1, r_2 \in (0.1, 0.9)$. Indeed note that R diverges for $r_1 \to 1$ and a fixed value of r_2, and for r_1 fixed and $r_2 \to 0$. The are two regions: for $r_2 > r_1$ we have $R < 1$, while for $r_2 < r_1$, we have $R > 1$. In the transition region, where $r_1 = r_2$, R is constantly equal to 1.

The particular cases can be discriminated using the following factorizations. Note that

$$\begin{aligned} a+c &= \cos^2\tilde{r}_1\sin^2\tilde{r}_2(1+\cos\tilde{\alpha}_1) - \sin^2\tilde{r}_1\cos^2\tilde{r}_2(1+\cos\tilde{\alpha}_2) \\ &= -\sin^2\tilde{r}_1\cos^2\tilde{r}_2\left[(1+\cos\tilde{\alpha}_2) - R^2(1+\cos\tilde{\alpha}_1)\right], \end{aligned} \tag{5.3.34}$$

and

$$\begin{aligned} b &= -\left[\cos^2\tilde{r}_1\sin^2\tilde{r}_2\sin\tilde{\alpha}_1 + \sin^2\tilde{r}_1\cos^2\tilde{r}_2\sin\tilde{\alpha}_2\right] \\ &= -\sin^2\tilde{r}_1\cos^2\tilde{r}_2\left[\sin\tilde{\alpha}_2 + R^2\cos\tilde{\alpha}_1\right]. \end{aligned} \tag{5.3.35}$$

Using (5.3.25), (5.3.34) and (5.3.35), we have the following:

1. $a+c=0$ whenever any of the following conditions are met:
   (a) $r_1 = 1$.
   (b) $r_2 = 0$.
   (c) $R = \sqrt{(1+\cos\tilde{\alpha}_2)/(1+\cos\tilde{\alpha}_1)}$.
2. $b=0$ whenever any of the following conditions are met:
   (a) $r_1 = 1$.
   (b) $r_2 = 0$.
   (c) $R = \sqrt{-\sin\tilde{\alpha}_2/\cos\tilde{\alpha}_1}$.
3. $\Delta = 0$ whenever any of the following conditions are met:
   (a) $r_1 = 0$ or $r_1 = 1$.
   (b) $r_2 = 0$ or $r_2 = 1$.
   (c) $\alpha_1 + \alpha_2 + p$ is an integer multiple of π.

For the general case ($a+c\neq 0$), u is obtained from (5.3.32) with $u=\tan k$, which gives

$$\tan k = \frac{\sin\tilde{\alpha}_2 + R^2\sin\tilde{\alpha}_1}{(1+\cos\tilde{\alpha}_2) - R^2(1+\cos\tilde{\alpha}_1)} \pm \frac{2R|\sin\frac{\tilde{\alpha}_1+\tilde{\alpha}_2}{2}|}{(1+\cos\tilde{\alpha}_2) - R^2(1+\cos\tilde{\alpha}_1)}. \tag{5.3.36}$$

Since our domain is $[-\pi,\pi]$, there are two lines which cut the branches of the tangent function, so we find two pairs of solutions, one corresponding to each sign choice in the original equation. It is worth noting that compatibility with (5.3.26) implies that solutions $k^*\in\mathbb{T}$ should verify, for the choice $s=1$,

$$\mathrm{Sg}[\sin(\alpha_1 + p/2 + k^*)] = \mathrm{Sg}[\sin(\alpha_1 + p/2 - k^*)], \tag{5.3.37}$$

and for the choice $s=-1$,

$$\mathrm{Sg}[\sin(\alpha_1 + p/2 + k^*)] = -\mathrm{Sg}[\sin(\alpha_1 + p/2 - k^*)]. \tag{5.3.38}$$

Remark 5.5. We observe that solutions acquire a simple form in some special cases of interest. Assume that $r_1 = r_2 = r \in (0,1)$, and that $\cos\tilde{\alpha}_1 \neq \cos\tilde{\alpha}_2$, the other parameters kept arbitrary. In this case $R = 1$, and (5.3.36) simplifies to

$$\tan k = \frac{\sin\tilde{\alpha}_2 + \sin\tilde{\alpha}_1}{\cos\tilde{\alpha}_2 - \cos\tilde{\alpha}_1} \pm \frac{2|\sin\frac{\tilde{\alpha}_1+\tilde{\alpha}_2}{2}|}{\cos\tilde{\alpha}_2 - \cos\tilde{\alpha}_1}. \tag{5.3.39}$$

We note in this case that the location of the critical points becomes independent of r.

A second interesting case is that in which each free QW has the same (non-trivial) coin, i.e. $r_1 = r_2 = r \in (0,1)$ and $\alpha_1 = \alpha_2 = \alpha$. Then from (5.3.24a)-(5.3.24c), both $c = 0$ and $a = 0$, and Lemma (5.2) implies that the critical values are the set $\{\pm\pi, \pm\pi/2, 0\}$. Using conditions (5.3.37) and (5.3.38), we find further that $\{0, \pm\pi\}$ are the critical points of $\lambda_{1,\pm}(k)$, and that $\{\pm\pi/2\}$ are those of $\lambda_{2,\pm}(k)$. It is remarkable that in this case the critical points turn out to be independent not only of r but also of α, in contrast to the one-dimensional case (cf. Eq. (5.3.6)).

5.3.3.2 Eigenvectors

The eigenvectors of $\hat{U}_0(k)$ are constructed via tensor product of the one-dimensional case, which was discussed in paragraph 5.3.2.4. For $j = 1, 2$, recall that ω_j are given by (5.3.19), and let

$$|v_{j,\pm}(k)\rangle = \frac{1}{\sqrt{2N_{j,\pm}(k)}} \left(e^{\mathrm{i}(\gamma_j - k)}, \frac{\pm\sin\omega_j(k) + r_j\sin(\alpha_j + k)}{\sqrt{1 - r_j^2}} \right)^{\mathrm{T}}, \tag{5.3.40}$$

and

$$N_{j,\pm}(k) = \frac{\sin\omega_j(k)}{1 - r_j^2} \left(\sin\omega_j(k) \pm r_j \sin(\alpha_j + k) \right). \tag{5.3.41}$$

The normalized eigenvectors with the corresponding sign choices are presented in Table 5.3.1.

Eigenvalue $\times e^{-\mathrm{i}\theta}$	Eigenvector
$\lambda_{1,+}(k) = e^{\mathrm{i}(\omega_1+\omega_2)}$	$\lvert u_{1,+}(k)\rangle := \lvert v_{1,+}(p/2+k)\rangle \otimes \lvert v_{2,+}(p/2-k)\rangle$
$\lambda_{1,-}(k) = e^{-\mathrm{i}(\omega_1+\omega_2)}$	$\lvert u_{1,-}(k)\rangle := \lvert v_{1,-}(p/2+k)\rangle \otimes \lvert v_{2,-}(p/2-k)\rangle$
$\lambda_{2,+}(k) = e^{\mathrm{i}(\omega_1-\omega_2)}$	$\lvert u_{2,+}(k)\rangle := \lvert v_{1,+}(p/2+k)\rangle \otimes \lvert v_{2,-}(p/2-k)\rangle$
$\lambda_{2,-}(k) = e^{-\mathrm{i}(\omega_1-\omega_2)}$	$\lvert u_{2,-}(k)\rangle := \lvert v_{1,-}(p/2+k)\rangle \otimes \lvert v_{2,+}(p/2-k)\rangle$

Table 5.3.1: Normalized eigenvectors of $\hat{U}_0(k) \in \mathcal{M}_4(\mathbb{C})$.

Example 5.3.2. The Hadamard walk corresponds to $r_1 = r_2 = \frac{1}{\sqrt{2}}$, $\alpha_1 = \alpha_2 = \frac{3\pi}{2}$, and $\theta_1 = \theta_2 = \frac{3\pi}{2}$, thus $\theta = \pi$. The one-dimensional case was studied in Example 5.3.1. Using the shorthand $k_{1,2} = p/2 \pm k$, and $j = 1, 2$, we find that

$$\lambda_{j,\pm}(k) = \frac{1}{2}\left(\pm\sqrt{1+\cos^2 k_1} - \mathrm{i}\sin k_1\right)\left(\pm(-1)^{j+1}\sqrt{1+\cos^2 k_2} - \mathrm{i}\sin k_2\right),$$

and the normalized eigenvectors are

$$|u_{j,\pm}\rangle = \frac{1}{2\sqrt{N'_{j,\pm}(k)}}\begin{pmatrix} e^{-\mathrm{i}k_1} \\ \pm\sqrt{1+\cos^2 k_1} - \cos k_1 \end{pmatrix} \otimes \begin{pmatrix} e^{-\mathrm{i}k_2} \\ \pm(-1)^{j+1}\sqrt{1+\cos^2 k_2} - \cos k_2 \end{pmatrix}$$

where

$$N'_{j,\pm}(k) = N_\pm(p/2+k)N_{\pm(-1)^{j+1}}(p/2-k), \tag{5.3.42}$$

and

$$N_\pm(k) = 1 + \cos^2 k \pm \cos k\sqrt{1+\cos^2 k}. \tag{5.3.43}$$

Note that $N_\pm(k) \neq 0$ for $k \in \mathbb{T}$. Indeed, if $k \notin \{\frac{n\pi}{2}\}_{n=0\ldots3}$, then

$$N_\pm(k) > \sqrt{1+\cos^2 k}\,(1 \pm \cos k) > 0. \tag{5.3.44}$$

The other cases are positive, $N_\pm(0) = N_\mp(\pi) = 2 \pm \sqrt{2}$, $N_\pm(\frac{\pi}{2}) = N_\pm(\frac{3\pi}{2}) = 1$.

5.4 Absence of singular continuous spectrum of the IQW

In this section we determine the spectral components of the IQW. This is achieved applying spectral stability arguments. In particular we explore the assumption of the interaction being p-summable, that is, $(I - \mathcal{V})$ belonging to a p-Schatten class of operators, since this is a suitable setting for perturbation theory.

5.4.1 The IQW as a perturbation problem

We will make use of the following elementary lemma characterizing multiplication operators in sequence spaces.

Lemma 5.3. *Consider a sequence of matrices $\{A(x)\}_{x\in\mathbb{Z}} \subset \mathcal{M}_d(\mathbb{C})$, such that $A(x) \to 0$ when $|x| \to \infty$, and let $\mathcal{A} \in \mathcal{L}(\mathcal{H})$ be the associated multiplication operator in $\mathcal{H} = \ell^2(\mathbb{Z}) \otimes \mathbb{C}^d$, i.e. $(\mathcal{A}\psi)(x) = A(x)\psi(x)$ for all $x \in \mathbb{Z}$, $\psi \in \mathcal{H}$. Let $p \geq 1$. Then $\mathcal{A}$ is in the p-Schatten class $\mathfrak{S}_p(\mathcal{H})$ if and only if $\{||A(x)||_F\}_{x\in\mathbb{Z}} \in \ell^p(\mathbb{Z})$.*

Proof. The condition $\lim_{|x|\to\infty} A(x) \to 0$ implies that $\mathcal{A}$ is compact. In fact it suffices to consider, for a fixed $N \geq 0$, the operator $(\mathcal{A}_N\psi)(x) := (\mathcal{A}\psi)(x) = A(x)\psi(x)$ if $|x| \leq N$ and zero otherwise. Since $\mathcal{A}$ is the norm limit of $\mathcal{A}_N$, which is of finite rank, $\mathcal{A}$ is compact.

The adjoint of $\mathcal{A}$ is $(\mathcal{A}^*\psi)(x) = A^\dagger(x)\psi(x)$. This is seen by computing

$$\langle\psi, A\psi\rangle = \sum_x \psi^\dagger(x)A(x)\psi(x) = \sum_x \left[\psi^\dagger(x)(A^\dagger(x)\psi(x))\right]^\dagger = \overline{\langle\psi, A^\dagger\psi\rangle} = \langle A^\dagger\psi, \psi\rangle.$$

Now, since $\sigma(\mathcal{A}^*\mathcal{A}) = \overline{\{\cup_{j=1}^d \lambda_j(A^\dagger(x)A(x)) : x \in \mathbb{Z}\}}$,

$$||\mathcal{A}||^p_{\mathfrak{S}_p(\mathcal{H})} = \sum_{x,j} s_j^p(A(x)) = \sum_x ||A(x)||_p^p. \tag{5.4.1}$$

Since the norms $||\cdot||_F$ and $||\cdot||_p$ are equivalent, there exist constants c_1 and c_2 such that $c_1||A(x)||_p \leq ||A(x)||_F \leq c_2||A(x)||_p$, and this allows to conclude.

□

Let us now express the IQW as a perturbation problem in the relative momentum coordinate. Recall that the dynamics for fixed total momentum p occurs in the Hilbert space $\mathcal{H}_{2,p} \simeq \ell^2(\mathbb{Z}) \otimes \mathbb{C}^4$, and the reciprocal space is $\hat{\mathcal{H}}_{2,p} \simeq L^2(\mathbb{T}) \otimes \mathbb{C}^4$. Let $\mathcal{U} = \mathcal{U}_0\mathcal{V}$ be written as

$$\mathcal{U} - \mathcal{U}_0 = -\mathcal{U}_0(I - \mathcal{V}). \tag{5.4.2}$$

Recall that the sequence $\{\Delta(x) : x \in \mathbb{Z}\}$ was defined as $\Delta(x) = ||I_4 - V(x)||_F^p$ for $x \in \mathbb{Z}$, though it is only relevant over one side (say, $\mathbb{N}$), because under the radial assumption, V is an even function of the relative coordinate x.

Proposition 5.5. *Under Assumption **(H0)**, the operator $(I - \mathcal{V})$ is compact. Additionally, $(I - \mathcal{V}) \in \mathfrak{S}_p$ for some $p \geq 1$ if and only if the series $\sum\limits_{x=1}^{\infty} \Delta^p(x)$ converges.*

Proof. Since $(I-\mathcal{V})$ is the multiplication operator by the sequence $\{I_4-V(x)\}_{x\in\mathbb{Z}}$, Lemma 5.3 applies. Note that evaluating only one side of the series is enough because $V(x)$ is an even function of x. □

We turn to the stability of the essential spectrum. In section 3 we proved that the spectrum of $\mathcal{U}_0$ is purely essential, i.e. $\sigma(\mathcal{U}_0) = \sigma_{ess}(\mathcal{U}_0)$. More precisely, it consists in two degenerate pairs of bands, $\sigma(\mathcal{U}_0) = \bigcup_{i=1}^{2}(B_{i,+} \cup B_{i,-})$, where $B_{i,+} = B_{i,-} = [\mu_i, \mu_i'] \subset \mathbb{S}$ for $i = 1, 2$. We are now in a position to apply classical perturbation theory arguments, which allow to arrive at the following theorem.

Theorem 5.1. *Assume that the IQW satisfying Assumption **(H0)** is, additionally, p-summable for some $p \geq 1$. Then:*

1. *the essential spectrum is stable, i.e. $\sigma_{ess}(\mathcal{U}) = \sigma_{ess}(\mathcal{U}_0)$, and*

2. *if the IQW is of trace class, i.e. $p = 1$, then $\sigma_{ac}(\mathcal{U}) = \sigma_{ac}(\mathcal{U}_0)$.*

Proof. (i) From the p-summability condition, we know from Lemma 5.3 that $(I - \mathcal{V}) \in \mathfrak{S}_p$, and in particular is compact. The stability condition criteria of Weyl under compact perturbations allows to conclude.

(ii) Since $(I - \mathcal{V}) \in \mathfrak{S}_1$, the claim follows from the Birman-Krein theorem on invariance of the absolutely continuous spectrum under trace-class perturbations, see [BK62] and references in [Joy94]. □

Under p-summability, the spectrum of $\mathcal{U}$ is the disjoint union of $\sigma_{ess}(\mathcal{U}_0)$ and $\sigma_d(\mathcal{U})$, the latter being an (at most countable) set of isolated eigenvalues of finite algebraic multiplicity, and they can only accumulate at $\sigma_{ess}(\mathcal{U}_0)$, which is a closed set.

Now we move on to study the singular continuous spectrum of the perturbed operator. In particular, we are interested in knowing under which conditions $\sigma_{sc}(\mathcal{U})$ is empty or not.

5.4.2 Absence of singular continuous spectrum

Recently, in [ABJ15] the authors derive sufficient conditions for a (possibly inhomogeneous) QW to have some nice spectral properties, using methods of unitary Mourre theory. They introduce the notion of *regularity* of a coin operator.

Definition 5.3 (see [ABJ15]). *The interaction $\mathcal{V} = \{V(x) \in U(4) : x \in \mathbb{Z}\}$ is said to be* regular *if*

$$\int_1^\infty \sup_{\lceil ar \rceil \le x \le \lfloor br \rfloor} \Delta(x)\, \mathrm{d}r < \infty, \tag{5.4.3}$$

for some constants $0 < a < b < \infty$.

Recall that the floor and ceiling functions map a real number to the largest previous or the smallest following integer, respectively. More precisely, for $r \in \mathbb{R}$, $\lceil r \rceil = \min\{x \in \mathbb{N} : x \ge r\}$ and $\lfloor r \rfloor = \max\{x \in \mathbb{N} : x \le r\}$. Given arbitrary $a, b \in \mathbb{R}^+$ with $0 < a < b < \infty$, consider the step functions $L(r) = \lceil ar \rceil$ and $R(r) = \lfloor br \rfloor$, which define the borders of the moving window appearing in the integral (5.4.3) for each $r \ge 1$. It may happen that $R(r)$ is smaller than $L(r)$ for some values of r, but since $b > a$, from some point on $R(r)$ will be greater, that is, the function

$$\chi_{a,b}(r) = \begin{cases} 1 & \text{if } L(r) \le R(r) \\ 0 & \text{otherwise} \end{cases} \tag{5.4.4}$$

satisfies $\chi_{a,b}(r) = 1$ for sufficiently large r, as proved below. We plot some examples in Fig. 5.4.1.

Note that we can multiply the integrand in (5.4.3) by $\chi_{a,b}(r)$ and the value of the integral remains the same, because $\chi_{a,b}(r)$ is either zero when then there are no points in the window to evaluate, or one otherwise.

Lemma 5.4. *The following piecewise formulas hold:*

$$L(r) = \begin{cases} \lceil a \rceil & \text{if } 1 \le r \le \frac{\lceil a \rceil}{a} \\ \lceil a \rceil + n & \text{if } \frac{\lceil a \rceil + n - 1}{a} < r \le \frac{\lceil a \rceil + n}{a},\ n \ge 1 \end{cases} \tag{5.4.5}$$

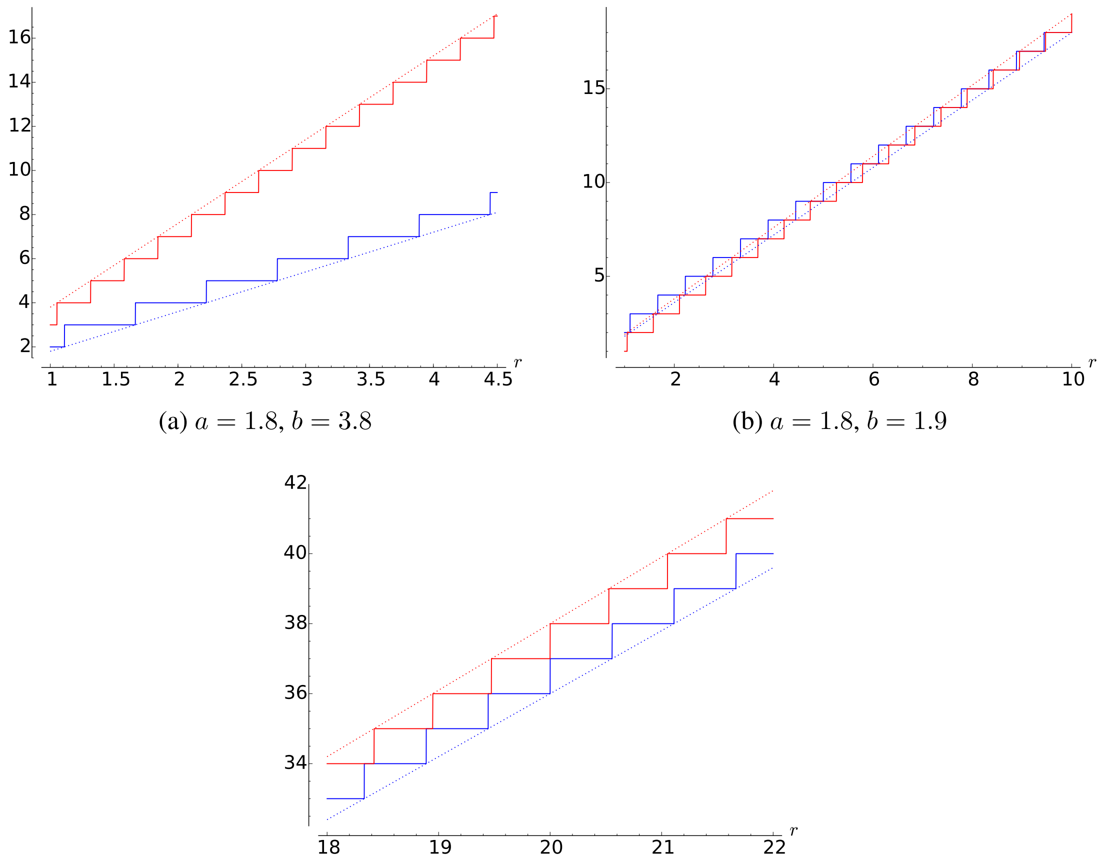
and

$$R(r) = \begin{cases} \lfloor b \rfloor & 1 \le r < \frac{\lfloor b \rfloor + 1}{b} \\ \lfloor b \rfloor + n & \frac{\lfloor b \rfloor + n}{b} \le r < \frac{\lfloor b \rfloor + n + 1}{b},\ n \ge 1 \end{cases}. \tag{5.4.6}$$

Moreover there exists r_0 such that

$$\chi_{a,b}(r) = 1 \qquad \forall r \ge r_0. \tag{5.4.7}$$

Proof. For (5.4.5), if $a \le ar \le \lceil a \rceil$, taking ceiling on each side gives $L(r) = \lceil a \rceil$; for the other piece take $n \ge 1$ and take ceiling on $\lceil a \rceil + n - 1 < ar \le \lceil a \rceil + n$, which gives $\lceil a \rceil + n - 1 < L(r) \le \lceil a \rceil + n$, and since there is only one integer on any half-open interval of length one, we must have $L(r) = \lceil a \rceil + n$.



(a) $a = 1.8$, $b = 3.8$

(b) $a = 1.8$, $b = 1.9$

(c) $a = 1.8$, $b = 1.9$, in the region when they start to separate

Figure 5.4.1: In blue (resp. red), $L(r)$, (resp. $R(r)$).

We proceed analogously for (5.4.6). If $b \leq br < \lfloor b \rfloor + 1$, taking floor on each side gives $\lfloor b \rfloor \leq R(r) < \lfloor b \rfloor + 1$, thus $R(r) = \lfloor b \rfloor$; for the general piece take $n \geq 1$ and taking floor over $\lfloor b \rfloor + n \leq br < \lfloor b \rfloor + n + 1$, gives $R(r) = \lfloor b \rfloor + n$.

Let us prove (5.4.7). For $r > \max\{\frac{\lceil a \rceil}{a}, \frac{\lfloor b \rfloor + 1}{b}\}$, from (5.4.5)-(5.4.6) there are integers n_1, n_2, both greater or equal than one, such that $L(r) = \lceil a \rceil + n_1(r)$ and $R(r) = \lfloor b \rfloor + n_2(r)$. Using that $n_1(r) < ar - \lceil a \rceil + 1$ and $n_2(r) > br - \lfloor b \rfloor - 1$, then

$$\begin{aligned} R(r) - L(r) &= \lfloor b \rfloor - \lceil a \rceil + n_2(r) - n_1(r) \\ &\geq -1 + n_2(r) - n_1(r) \\ &> -1 + (br - \lfloor b \rfloor - 1) - (ar - \lceil a \rceil + 1) \\ &= (b-a)r - 3 + (\lceil a \rceil - \lfloor b \rfloor). \end{aligned} \tag{5.4.8}$$

Let us show that $\frac{3+\lfloor b\rfloor-\lceil a\rceil}{b-a} > \frac{\lfloor b\rfloor+1}{b}$:

$$\begin{aligned}\frac{3+\lfloor b\rfloor-\lceil a\rceil}{b-a}-\frac{\lfloor b\rfloor+1}{b} &\geq \frac{2+b-\lceil a\rceil}{b-a}-\frac{b+1}{b} \\ &\geq \frac{b+ab+a-b\lceil a\rceil}{(b-a)b} \geq \frac{a}{(b-a)b} > 0. \end{aligned} \tag{5.4.9}$$

We conclude from (5.4.8), that that $R(r)-L(r)>0$ is fulfilled if

$$r > r_0 := \max\left\{\frac{\lceil a\rceil}{a}, \frac{3+\lfloor b\rfloor-\lceil a\rceil}{b-a}\right\}. \tag{5.4.10}$$

□

After these preliminaries, we investigate the relationship between regularity and summability of the interaction.

Proposition 5.6. *Consider a radial interaction $\mathcal{V}=\{V(x)\in U(4) : x\in\mathbb{Z}\}$. If $\{\Delta(x)\}_{x\in\mathbb{N}}$ is a monotonically decreasing sequence, then regularity is equivalent to convergence of the series $\sum_{x\in\mathbb{N}}\Delta(x)$.*

Proof. Taking r_0 from Lemma 5.4,

$$\begin{aligned}\int_1^\infty \sup_{\lceil ar\rceil\leq x\leq\lfloor br\rfloor}\Delta(x)\chi_{a,b}(r)\,\mathrm{d}r &= c_1+\int_{r_0}^\infty \sup_{\lceil ar\rceil\leq x\leq\lfloor br\rfloor}\Delta(x)\,\mathrm{d}r \\ &= c_1+c_2+\frac{1}{a}\sum_{i=1}^\infty \Delta(\lceil a\rceil+i),\end{aligned}$$

with $c_1<\infty$, and from (5.4.5) we know that $0<c_2\leq\frac{\Delta(\lfloor ar_0\rfloor)}{a}$. The claim follows. □

In the general case the conditions of regularity and trace-class are no longer equivalent. In fact as we show below, the regularity condition is stronger.

Proposition 5.7. *Consider a radial interaction $\mathcal{V}=\{V(x)\in U(4) : x\in\mathbb{Z}\}$.*

(i) If $\mathcal{V}$ is regular, then $\sum_{x\in\mathbb{N}}\Delta(x)$ converges.

(ii) The converse of the previous assertion is not true in general.

Proof. (i) Taking r_0 from Lemma 5.4,

$$\begin{aligned}\int_1^\infty \sup_{\lceil ar\rceil\leq x\leq\lfloor br\rfloor}\Delta(x)\chi_{a,b}(r)\,\mathrm{d}r &\geq \int_{r_0}^\infty \sup_{\lceil ar\rceil\leq x\leq\lfloor br\rfloor}\Delta(x)\,\mathrm{d}r \\ &\geq \int_{r_0}^\infty \Delta(\lfloor br\rfloor)\mathrm{d}r \\ &= c+\frac{1}{b}\sum_{i=1}^\infty \Delta(\lfloor br_0\rfloor+i),\end{aligned}$$

where $0 < c \leq \frac{\Delta(\lfloor b r_0 \rfloor)}{b}$. By contradiction, assume that $\sum_{x=1}^{\infty} \Delta(x)$ diverges. Then from the inequality above, the integral diverges, because an infinite subset of a divergent series of positive terms diverges.

(ii) We build a counterexample. Let $a = 1$, $b = 2$. From (5.4.5)-(5.4.6), for $n \in \mathbb{N}_0$, $L(r) = 1 + n$ if $n < r \leq n + 1$, and $R(r) = 2 + n$ for $1 + n/2 \leq r < 3/2 + n/2$. Then

$$\begin{aligned} \int_1^{\infty} \sup_{L(r) \leq x \leq R(r)} \Delta(x) \mathrm{d}r &= \sum_{n=1}^{\infty} \int_n^{n+1} \sup_{L(r) \leq x \leq R(r)} \Delta(x) \mathrm{d}r \\ &= \frac{1}{2} \sum_{n=1}^{\infty} \left(\sup_{n+1 \leq x \leq 2n} \Delta(x) + \sup_{n+1 \leq x \leq 2n+1} \Delta(x) \right). \end{aligned} \tag{5.4.11}$$

Let us rewrite the last series as

$$\begin{aligned} &\left(\sup_{2 \leq x \leq 2} \Delta(x) + \sup_{2 \leq x \leq 3} \Delta(x) \right) + \left(\sup_{3 \leq x \leq 4} \Delta(x) + \sup_{3 \leq x \leq 5} \Delta(x) + \sup_{4 \leq x \leq 6} \Delta(x) + \sup_{4 \leq x \leq 7} \Delta(x) \right) \\ &+ \left(\sup_{5 \leq x \leq 8} \Delta(x) + \sup_{5 \leq x \leq 9} \Delta(x) + \ldots + \sup_{8 \leq x \leq 14} \Delta(x) + \sup_{8 \leq x \leq 15} \Delta(x) \right) + \ldots \\ &= \sum_{n=1}^{\infty} \sum_{k=0}^{2^n - 1} \sup \left\{ \Delta(x) \quad : 2^{n-1} + 1 + \left\lfloor \frac{k}{2} \right\rfloor \leq x \leq 2^n + k \right\}. \end{aligned} \tag{5.4.12}$$

The idea is that each term in parentheses shares the same power of two, if we look at all the intervals which appear in the sum.

Now, given $c > 1$, consider the sequence $\{x_n = c^n\}_{n \in \mathbb{N}}$, and let

$$\Delta(x) = \begin{cases} c^{-n} & \text{if } x = x_n, \\ 0 & \text{otherwise .} \end{cases} \tag{5.4.13}$$

Clearly,

$$\sum_{x=1}^{\infty} \Delta(x) = \sum_{n=1}^{\infty} \Delta(x_n) = 1/(c-1) = 1 < \infty. \tag{5.4.14}$$

Let $c = b/a = 2$. Using (5.4.12)-(5.4.13) in (5.4.11), we arrive at

$$\begin{aligned} \int_1^{\infty} \sup_{L(r) \leq x \leq R(r)} \Delta(x) \mathrm{d}r &= \frac{1}{2} \sum_{n=1}^{\infty} \sum_{k=0}^{2^n - 1} \Delta(2^n) \\ &= \frac{1}{2} \sum_{n=1}^{\infty} 2^n \Delta(2^n) = \frac{1}{2} \sum_{n=1}^{\infty} 1, \end{aligned} \tag{5.4.15}$$

which diverges.

□

Applying Corollary 4.5 of [ABJ15], we obtain the following result.

Corollary 5.1. *Consider an IQW, assume that hypothesis **(H0)** holds, and that the interaction is trace-class and monotonically decreasing. Then*

$$\sigma_{ac}(\mathcal{U}) = \sigma_{ac}(\mathcal{U}_0), \qquad \sigma_{sc}(\mathcal{U}) = \emptyset, \tag{5.4.16}$$

and the eigenvalues of $\mathcal{U}$ *are either a finite set or an infinite set which can accumulate only at the edges of the bands.*

5.5 Lieb-Thirring type estimates

It often happens that the exact determination of the spectrum an operator is a hard task. However a valuable alternative task is to relate the behaviour of sums or weighted sums of the eigenvalues, with properties of the behaviour of functions of the coefficients of the problem at hand[4].

Inequalities of the Lieb-Thirring type, first appeared at the end of the seventies (see collected works here [LT02]), were attempted to provide a rigorous proof of the stability of matter [LS10]. In the form that we will present them, they give information about how fast the eigenvalues approach the bands of the continuous spectrum. We should remark that they do not say nothing about the *existence* of eigenvalues, but rather the bounds apply in any circumstance, be there none, a finite or an infinite number. In this sense, this section is complementary to the eigenvalue problem presented in Section 5.6, where we the problem of existence of eigenvalues is addressed.

5.5.1 Discrete eigenvalue estimates I

In finite dimensional spaces, a classical estimate giving information about the change in the eigenvalues for some change in the matrix is the Hoffman-Wielandt inequality [HW$^+$53]. See [Bha97] Chapter VI for proofs and further details.

Theorem 5.2. *(Hoffman-Wielandt inequality) Let* $A, B \in \mathcal{M}_n(\mathbb{C})$ *be normal matrices, with eigenvalues* $\{\lambda_1, \dots, \lambda_n\}$ *and* $\{\mu_1, \dots \mu_n\}$ *respectively. Then*

$$\min_{\sigma \in S_n} \left(\sum_{i=1}^{n} |\lambda_i - \mu_{\sigma(i)}|^2 \right)^{1/2} \leq ||A - B||_F \leq \max_{\sigma \in S_n} \left(\sum_{i=1}^{n} |\lambda_i - \mu_{\sigma(i)}|^2 \right)^{1/2}, \tag{5.5.1}$$

where S_n *is the set of permutations on* n *symbols.*

The extension to infinite dimensional Hilbert spaces of the Hoffman-Wielandt inequality was achieved by Kato [Kat87] for the case of a pair of self-adjoint operators which differ in a compact operator. It was subsequently generalized in [BS88] for unitary operators with compact difference, in [BE94] for a pair of normal operators with Hilbert-Schmidt difference, and in [EF95] for a pair of normal operators with Hilbert-Schmidt difference. More recently, Hansmann et al. [Han11, Han13] developed a powerful method of perturbation

[4] Cf. *"spectral gems"*, quoting Barry Simon [Sim09].

determinant and complex analysis, which can be applied to general bounded operators, see [Han10] for further details.

Let us first apply the result for a pair of unitary operators to the IQW. We need to introduce the notion of an *extended enumeration* of the discrete eigenvalues. If U is a unitary operator, an extended enumeration of its eigenvalues is a sequence of complex numbers $\{\mu_j\}$ such that any discrete eigenvalue of U of multiplicity m appears in the sequence exactly m times, and any other element of the sequence is a boundary point of the essential spectrum (with respect to $\partial\mathbb{D}$).

Theorem 5.3 (see [BS88])**.** *Let U, V be unitary operators in $\mathcal{H}$ such that their difference $C = U - V$ is in $\mathfrak{S}_p(\mathcal{H})$ for some $1 \leq p \leq \infty$. Then there exist extended enumerations $\{\mu_j\}$, $\{\nu_j\}$ of discrete eigenvalues of U,V respectively, such that*

$$\sum_j |\mu_j - \nu_j|^p \leq \left(\frac{\pi}{2}\right)^p ||C||^p_{\mathfrak{S}_p}. \tag{5.5.2}$$

Moreover, the constant $\pi/2$ occurring in the above inequality cannot be replaced by a smaller constant: for $p = 1$, the estimate is sharp.

Using this result we can directly obtain an estimate for the discrete eigenvalues of the IQW. Recall that $\sigma(\mathcal{U}_0) = \sigma_{ess}(\mathcal{U}_0) = B_{1,+} \cup B_{1,-} \cup B_{2,+} \cup B_{2,-}$, and that their edges are denoted $B_{1,+} = [\mu_1, \mu_1']$, etc.; the subindex in the μ_i's can be dropped because $B_{1,+} = B_{1,-}$ and $B_{2,+} = B_{2,-}$.

Corollary 5.2. *Consider an IQW satisfying* **(H0)**, *and suppose it is p-summable for some $p \geq 1$. Then, the following estimate holds:*

$$\sum_{e^{\mathrm{i}\omega} \in \sigma_d(\mathcal{U})} \mathrm{dist}(e^{\mathrm{i}\omega}, \sigma(\mathcal{U}_0))^p \leq c_p \sum_{x\in\mathbb{Z}} \Delta(x)^p, \tag{5.5.3}$$

with $c_p > 0$ a constant independent of $\mathcal{V}$ and which depends only on p.

Proof. We apply Theorem 5.3 for $p = 1$. Since any extended enumeration of $\mathcal{U}_0$ is a (possibly infinite) sequence containing only the extremes of the bands, the only non-vanishing terms of the sum are obtained choosing $e^{\mathrm{i}\omega} \in \sigma_d(\mathcal{U})$. Taking the minimum over all possible choices guarantees that the existence bound (5.5.2) can be applied. We have that

$$\mathrm{dist}(e^{\mathrm{i}\omega}, \sigma(\mathcal{U}_0))^p = \min_{1\leq i\leq 2}\{|e^{\mathrm{i}\omega} - \mu_i|^p, |e^{\mathrm{i}\omega} - \mu_i'|^p\}. \tag{5.5.4}$$

In terms of $\Delta(x) = ||I_4 - V(x)||_F = ||I_4 - V(x)||_{\mathfrak{S}_2}$, from equivalence of norms there is a constant $c_p > 0$ such that the right-hand side of (5.5.3) is

$$\left(\frac{\pi}{2}\right)^p ||I - \mathcal{V}||^p_{\mathfrak{S}_p} = \left(\frac{\pi}{2}\right)^p \sum_x ||I_4 - V(x)||^p_p \leq c_p \sum_{x\in\mathbb{Z}} \Delta(x)^p. \tag{5.5.5}$$

□

5.5.2 Discrete eigenvalue estimates II

The following result, due to Hansmann [Han13], is an application to unitary operators of estimation of discrete spectra. It applies to the Schatten classes $p > 1$.

Theorem 5.4 (see [Han13] Th. 2)**.** *Let $U \in \mathcal{L}(\mathcal{H})$ be unitary and $\sigma(U) \neq \mathbb{T}$. Let $V \in \mathcal{L}(\mathcal{H})$, such that $V - U \in \mathfrak{S}_p(\mathcal{H})$ for some $p > 1$. Let $\tau \in \mathbb{T} \setminus (\sigma(U) \cup \sigma(V))$. Then*

$$\sum_{\lambda \in \sigma_d(V)} \frac{\operatorname{dist}(\lambda, \sigma(U))^p}{|\tau - \lambda|^p} \leq c_p ||(V - \tau I)^{-1} - (U - \tau I)^{-1}||^p_{\mathfrak{S}_p}, \tag{5.5.6}$$

where $c_p > 0$ is a constant which depends only on p.

Note that the previous estimate involves a weighted sum respect to a point $\tau \in \mathbb{T}$ that is not in the spectrum of $\mathcal{U}$. Such τ always exists provided that we exclude the trivial cases (either r_1 or r_2 belong to the edges of $[0, 1]$). Also recall that $\sigma(\mathcal{U}_0) \subset \sigma(\mathcal{U})$. In our setting, we derive the following estimate.

Corollary 5.3. *Consider an IQW satisfying* **(H0)***, and assume that the interaction is p-summable for some $p > 1$. Let $\tau \in \mathbb{T} \setminus \sigma(\mathcal{U})$. Then*

$$\sum_{e^{\mathrm{i}\omega} \in \sigma_d(\mathcal{U})} \frac{\operatorname{dist}(e^{\mathrm{i}\omega}, \sigma(\mathcal{U}_0))^p}{|\tau - e^{\mathrm{i}\omega}|^p} \leq \frac{c_p}{\operatorname{dist}(\tau, \sigma(\mathcal{U}_0))^p \operatorname{dist}(\tau, \sigma(\mathcal{U}))^p} \sum_{x \in \mathbb{Z}} \Delta^p(x), \tag{5.5.7}$$

where $c_p > 0$ is a constant which depends only on p.

Proof. Since $\sigma(\mathcal{U}_0) \neq \mathbb{T}$, Theorem 5.4 applies, giving

$$\sum_{e^{\mathrm{i}\omega} \in \sigma_d(\mathcal{U})} \frac{\operatorname{dist}(e^{\mathrm{i}\omega}, \sigma(\mathcal{U}_0))^p}{|\tau - e^{\mathrm{i}\omega}|^p} \leq c_p ||R(\mathcal{U}, \tau) - R(\mathcal{U}_0, \tau)||^p_{\mathfrak{S}_p}. \tag{5.5.8}$$

When the resolvent of two operators is evaluated at the same point, we can factor their difference via the *second resolvent identity*, namely for $\tau \in \rho(\mathcal{U})$, we have that

$$\begin{aligned} R(\mathcal{U}, \tau) - R(\mathcal{U}_0, \tau) &= R(\mathcal{U}_0, \tau)(\mathcal{U}_0 - \tau I)R(\mathcal{U}, \tau) - R(\mathcal{U}_0, \tau)(\mathcal{U} - \tau I)R(\mathcal{U}, \tau) \\ &= R(\mathcal{U}_0, \tau) \left(\mathcal{U}_0 - \tau I - \mathcal{U} + \tau I\right) R(\mathcal{U}, \tau) \\ &= R(\mathcal{U}_0, \tau)(\mathcal{U}_0 - \mathcal{U})R(\mathcal{U}, \tau). \end{aligned}$$

Since $\mathcal{U}_0 - \mathcal{U} = \mathcal{U}_0(I - \mathcal{V})$, then

$$\begin{aligned} ||R(\mathcal{U}, \tau) - R(\mathcal{U}_0, \tau)||_{\mathfrak{S}_p} &= ||R(\mathcal{U}, \tau)\mathcal{U}_0(I - \mathcal{V})R(\mathcal{U}, \tau)||_{\mathfrak{S}_p} \\ &\leq ||R(\mathcal{U}_0, \tau)||\, ||I - \mathcal{V}||_{\mathfrak{S}_p} ||R(\mathcal{U}, \tau)|| \\ &\leq \frac{||I - \mathcal{V}||_{\mathfrak{S}_p}}{\operatorname{dist}(\tau, \sigma(\mathcal{U}_0)) \operatorname{dist}(\tau, \sigma(\mathcal{U}))}. \end{aligned} \tag{5.5.9}$$

In the last step we used that $\mathcal{U}$ and $\mathcal{U}_0$ are normal. To conclude we combine (5.5.8), (5.5.9) and equivalence of norms as in (5.5.5) (the constant c_p is generic).

□

Lastly, we note that for any $e^{\mathrm{i}\omega} \in \sigma_d(\mathcal{U})$ and $\tau \in \mathbb{T} \setminus \sigma(\mathcal{U})$,

$$\frac{1}{\max\limits_{1\le i\le 2}\{|\tau-\mu_i|, |\tau-\mu_i'|\}} \le \frac{1}{|\tau - e^{\mathrm{i}\omega}|} \le \frac{1}{\min\limits_{1\le i\le 2}\{|\tau-\mu_i|, |\tau-\mu_i'|\}}, \tag{5.5.10}$$

and consequently the term $|\tau - e^{\mathrm{i}\omega}|$ can be extracted from the sum (5.5.7), thus giving

$$\sum_{e^{\mathrm{i}\omega}\in\sigma_d(\mathcal{U})} \mathrm{dist}(e^{\mathrm{i}\omega}, \sigma(\mathcal{U}_0))^p \le c_p \frac{\max\limits_{1\le i\le 2}\{|\tau-\mu_i|^p, |\tau-\mu_i'|^p\}}{\mathrm{dist}(\tau,\sigma(\mathcal{U}_0))^p\,\mathrm{dist}(\tau,\sigma(\mathcal{U}))^p} \sum_{x\in\mathbb{Z}} \Delta^p(x). \tag{5.5.11}$$

Clearly, inequality (5.5.3) is related to (5.5.11) but the latter incorporates a τ-dependent coefficient that is expected to be greater than 1, so in this respect inequality (5.5.3) is better.

5.6 Eigenvalue problem

This section is devoted to the eigenvalue problem associated to the IQW in the relative momentum Hilbert space, $\hat{\mathcal{H}}_{rel.} = L^2(\mathbb{T};\mathbb{C}^4)$, i.e. the total momentum p is fixed. In Proposition 5.2 it was shown that the relevant object of study is the integral equation

$$(\hat{\mathcal{U}}\hat{\psi})(k) = \hat{U}_0(k)\cdot\frac{1}{2\pi}\int_{-\pi}^{\pi}\hat{V}(k-k')\hat{\psi}(k')\mathrm{d}k', \qquad k\in\mathbb{T}. \tag{5.6.1}$$

Since $\hat{\mathcal{U}}$ is a unitary operator, its eigenvalues lie on the unit circle $\mathbb{S} = \{z\in\mathbb{C} : |z| = 1\}$, and the eigenvalue problem is to solve

$$\hat{\mathcal{U}}\hat{\psi} = e^{\mathrm{i}\omega}\hat{\psi} \qquad \text{for some non-trivial } \hat{\psi}\in\hat{\mathcal{H}}_{rel.}. \tag{5.6.2}$$

The main difficulty posed by (5.6.1) is that it has a distributional kernel, and since it is not in general a regular function, the convolution integral is not a compact operator and standard methods do not apply straightforwardly. To tackle this problem we proceed in three steps. First, we show that decoupling the interaction at the contact point ($x = 0$) from long-range interactions, there is a new integral operator, with well-behaved kernel (under suitable hypothesis on the decay rate of the interaction). Second, we formally solve the eigenvalue problem via analytic Fredholm theory, and identify the objects which condition the existence of eigenvalues of the IQW. Third, we transform the eigenvalue problem (5.6.2) into an algebraic problem that is suitable for numerical computations.

5.6.1 Decoupling the integral equation at the contact point

The even and odd parts of V are

$$V(x) = \frac{V(x)+V(-x)}{2} + \frac{V(x)-V(-x)}{2} = V_e(x) + V_o(x). \tag{5.6.3}$$

Then

$$\hat{V}(k) = \sum_{x=-\infty}^{\infty} e^{-\mathrm{i}kx} V(x) = \sum_{x=-\infty}^{\infty} e^{-\mathrm{i}kx} \left(I_4 + V_e(x) - I_4 + V_o(x) \right)$$

$$= \sum_{x=-\infty}^{\infty} e^{-\mathrm{i}kx} I_4 \; - (I_4 - V(0)) - \sum_{x=1}^{\infty} 2(I_4 - V_e(x)) \cos kx - \mathrm{i} \sum_{x=1}^{\infty} 2V_o(x) \sin kx.$$

Assuming that V is radial, then it is an even function of the relative position x, implying that $V_o = 0$ and

$$\hat{V}(k) = 2\pi\delta(k) I_4 - D(0) - G(k), \tag{5.6.4}$$

with

$$G(k) := \sum_{x=1}^{\infty} 2D(x) \cos kx, \qquad D(x) = I_4 - V(x). \tag{5.6.5}$$

Remark 5.6. The series in (5.6.5) is convergent in general in the sense of distributions, because the general term is clearly a sequence of slow growth (using that V is vanishing at infinity). For a broad class of interactions, $G(k)$ is a regular function -in particular continuous in $\mathbb{T}$-. Let us assume, on top of **(H0)**, that $(I - \mathcal{V}) \in \mathfrak{S}_1$, which we saw in Corollary 5.5 that is equivalent to the series of general term $\Delta(x) = ||D(x)||_F$ being finite. A standard argument allows to conclude that $G_{ij}(k) \in C(\mathbb{T})$, $i, j = 1, \ldots, 4$. In fact, the Weierstrass M-test applies, since $||D(x) \cos kx||_F \leq \Delta(x)$ and the series $\sum_{x=1}^{\infty} \Delta(x)$ converges, hence the series in (5.6.5) converges uniformly on $\mathbb{T}$; by the uniform limit theorem, this limit is also a continuous function, since each $D(x) \cos kx$ is continuous in k. □

Let

$$N_0 \hat{\psi} := \frac{1}{2\pi} \int_{-\pi}^{\pi} \hat{\psi}(k) \mathrm{d}k = \psi(0) \tag{5.6.6}$$

denote the projection onto the zeroth component of the relative distance. Let $\mathcal{G}$ denote the integral operator in $\mathbb{T}$ with associated kernel G, i.e.

$$(\mathcal{G}\hat{\psi})(k) := \frac{1}{2\pi} \int_{-\pi}^{\pi} G(k - k') \hat{\psi}(k') \mathrm{d}k', \qquad k \in \mathbb{T}. \tag{5.6.7}$$

Making the corresponding substitutions into (5.6.1), we find that an eigenvector $\hat{\psi}$ of $\hat{\mathcal{U}}$ must sastify

$$e^{\mathrm{i}\omega} \hat{\psi} = \hat{\mathcal{U}}_0 \hat{\psi} - \hat{\mathcal{U}}_0 D(0) N_0 \hat{\psi} - \hat{\mathcal{U}}_0 \mathcal{G} \hat{\psi}, \tag{5.6.8}$$

which upon rearranging becomes

$$D(0) N_0 \hat{\psi} + \mathcal{G} \hat{\psi} = \hat{\mathcal{U}}_0^{-1} (\hat{\mathcal{U}}_0 - e^{\mathrm{i}\omega}) \hat{\psi}. \tag{5.6.9}$$

We have thus decoupled the interaction at the contact point, $x = 0$, with the term arising when the particles are at relative position $x > 0$. The non-local interactions information is contained in the integral equation with kernel $G(k)$. We stress that related works

[AAM+12] on IQWs have considered the contact interaction, that is, $\mathcal{G}$ identically zero (this important case is revisited in detail in Subsection 5.7.1). In the following sections we embark on the analysis of the general case given by (5.6.9).

5.6.2 Formal solution

In the following we shall work under the hypothesis that $\mathcal{G}$ is a compact operator. As already discussed in Remark 5.6, assuming that the IQW is trace-class guarantees that the kernel $G(k)$ is continuous on $\mathbb{T}$. In this situation $\mathcal{G}$ is indeed compact, as can be deduced from the following more general result.

Theorem 5.5 (see [GH10])**.** *Let $\mathcal{K}$ be a bounded linear operator in the Hilbert space $L^p(\mathbb{T}) \otimes \mathbb{C}^d$, $d \geq 1$, $1 \leq p \leq \infty$, given by the equality*

$$(\mathcal{K}\hat{\psi})(k) = \frac{1}{2\pi} \int_{-\pi}^{\pi} K(k - k')\hat{\psi}(k')\, \mathrm{d}k', \qquad k \in \mathbb{T}, \tag{5.6.10}$$

where $K(k) \in \mathcal{M}_d(L^q(\mathbb{T}; \mathbb{C}))$, $q \geq 1$. Then for every p the operator $\mathcal{K}$ is compact.

To go further it is convenient to make a couple of definitions. First, we define a modified resolvent $\mathcal{R}_0$ for $e^{\mathrm{i}\omega} \notin \sigma(\hat{\mathcal{U}}_0)$, $(\mathcal{R}_0(e^{\mathrm{i}\omega})\hat{\psi})(k) = R_0(e^{\mathrm{i}\omega}, k)\hat{\psi}(k)\ \forall \hat{\psi} \in \hat{\mathcal{H}}_{rel.}$, with

$$R_0(e^{\mathrm{i}\omega}, k) := (\hat{U}_0(k) - e^{\mathrm{i}\omega})^{-1}\hat{U}_0(k), \qquad k \in \mathbb{T}. \tag{5.6.11}$$

Remark 5.7. The object $\mathcal{R}_0(e^{\mathrm{i}\omega})$, instead of the resolvent itself, has already appeared in the context of perturbations of unitary operators, see for instance [KK70], [Joy94]. To see this more clearly, let us go back to the general picture and consider the problem $U = U_0V$, where U, U_0, V are unitary operators. Writing the eigenvalue problem $U\psi = \lambda\psi$ in the form $(U_0 - \lambda)\psi = U_0(I - V)\psi$, it is plain that $\psi = R_0(\lambda)(I - V)\psi$ for $\lambda \notin \sigma(U_0)$.

Second, we define

$$A(z) = \frac{1}{2\pi} \int_{\mathbb{T}} (I - \mathcal{R}_0(z)\mathcal{G})^{-1} R_0(z, k)\, \mathrm{d}k. \tag{5.6.12}$$

Note that $A(z) \in \mathcal{M}_4(\mathbb{C})$, and we are assuming that $z \notin \sigma(\hat{\mathcal{U}}_0)$ and that $(I - \mathcal{R}_0(z)\mathcal{G})^{-1} \in \mathcal{L}(\hat{\mathcal{H}}_{rel.})$. The validity of these hypothesis is discussed below. Here $R_0(z, k) = (\hat{U}_0(k) - z)^{-1}\hat{U}_0(k)$ analytically extends (5.6.11) to the region $\mathbb{C} \setminus \sigma(\hat{\mathcal{U}}_0)$ (by *region* we mean a connected and open set, which holds because $\sigma(\hat{\mathcal{U}}_0)$ is always closed[5]).

The formal solution of the eigenvalue problem (5.6.2) can be given as follows.

Theorem 5.6. *Consider an IQW with an interaction satisfying hypothesis **(H0)**, and that is also trace-class. Assume that for some $e^{\mathrm{i}\omega} \notin \sigma(\hat{\mathcal{U}}_0)$, the operator $(I - \mathcal{R}_0(e^{\mathrm{i}\omega})\mathcal{G})$ is invertible. Then, $e^{\mathrm{i}\omega} \in \sigma_p(\mathcal{U})$ if and only if*

$$1 \in \sigma\left(A(e^{\mathrm{i}\omega})D(0)\right). \tag{5.6.13}$$

[5] Of course connectedness holds provided that we avoid the trivial cases r_1 or $r_2 \in \{0, 1\}$, in which $\sigma(\hat{\mathcal{U}}_0) = \mathbb{S}$.

Proof. Since $e^{\mathrm{i}\omega} \notin \sigma(\hat{\mathcal{U}}_0)$, $\mathcal{R}_0$ is a well-defined bounded linear operator in $\hat{\mathcal{H}}_{rel.}$. Multiplying (5.6.9) from the left by $\mathcal{R}_0$, we obtain

$$\mathcal{R}_0(e^{\mathrm{i}\omega})D(0)N_0\hat{\psi} + \mathcal{R}_0(e^{\mathrm{i}\omega})\mathcal{G}\hat{\psi} = \hat{\psi}, \tag{5.6.14}$$

which is equivalent to

$$\mathcal{R}_0(e^{\mathrm{i}\omega})D(0)N_0\hat{\psi} = (I - \mathcal{R}_0(e^{\mathrm{i}\omega})\mathcal{G})\hat{\psi}. \tag{5.6.15}$$

Since by hypothesis $(I - \mathcal{R}_0(e^{\mathrm{i}\omega})\mathcal{G})$ is invertible,

$$\hat{\psi} = (I - \mathcal{R}_0(e^{\mathrm{i}\omega})\mathcal{G})^{-1}\mathcal{R}_0(e^{\mathrm{i}\omega})D(0)N_0\hat{\psi}. \tag{5.6.16}$$

Integrating in $\mathbb{T}$, and since $N_0\hat{\psi} = \psi(0)$, we get

$$\frac{1}{2\pi}\int_{\mathbb{T}} \hat{\psi}(k)\mathrm{d}k = \left[\frac{1}{2\pi}\int_{\mathbb{T}} (I - \mathcal{R}_0(e^{\mathrm{i}\omega})\mathcal{G})^{-1}R_0(e^{\mathrm{i}\omega}, k)\mathrm{d}k\right] D(0)\psi(0), \tag{5.6.17}$$

hence

$$\psi(0) = A(e^{\mathrm{i}\omega})D(0)\psi(0), \tag{5.6.18}$$

which holds for a non-trivial $\psi(0)$ if and only if Ker $(I - A(e^{\mathrm{i}\omega})D(0)) \neq \{0\}$, equivalently if and only if (5.6.13) holds.

□

The basic information about the existence or not of the inverse of $(I - \mathcal{R}_0(e^{\mathrm{i}\omega})\mathcal{G})$ is contained in the following standard result, known as the analytic[6] Fredholm alternative. As a preparation the following remark will be useful.

Remark 5.8. We continue assuming that the interaction is trace-class, thus $\mathcal{G}$ is compact from Theorem 5.5 and in particular $||\mathcal{G}||$ is finite, and consequently the operator $\mathcal{R}_0(z)\mathcal{G}$ is a compact analytic operator-valued function for each $z \in D$, with $D = \mathbb{C} \setminus \sigma(\hat{\mathcal{U}}_0)$ (recall that compact operators are a two-sided ideal in $\mathcal{L}(\mathcal{H})$). Here analyticity derives from the fact that the resolvent of any bounded linear operator is analytic in its resolvent set[7].

Theorem 5.7 (see [Yaf91], Ch. I, Sect. 8)**.** *Let $D \subset \mathbb{C}$ be a region and let $\mathcal{M}(z)$ be an analytic operator-valued function on D such that $\mathcal{M}(z)$ is a compact operator in a Hilbert space for each $z \in D$. Then, either:*

1. *$(I - \mathcal{M}(z))^{-1}$ exists for no $z \in D$; or*
2. *$(I - \mathcal{M}(z))^{-1}$ exists for all $z \in D \setminus D_0$, where D_0 is a discrete subset of D. In this case, $(I - \mathcal{M}(z))^{-1}$ is meromorphic[8] in D with possible poles belonging to D_0.*

[6]Recall that an operator-valued function $T(\lambda)$ which maps a subset of $\mathbb{C}$ into $\mathcal{L}(\mathcal{H})$ is *analytic* at λ_0 if $T(\lambda) = T_0 + (\lambda - \lambda_0)T_1 + (\lambda - \lambda_0)^2T_2 + \ldots$, and where each T_i is in $\mathcal{L}(\mathcal{H})$ and the series converges for each λ in some neighborhood of λ_0.

[7]See for instance [GGK03].

[8]Recall that a function f is said to be *meromorphic* in an open set $\Omega \subset \mathbb{C}$ if there is a set $\Omega_0 \subset \Omega$ such that: (i) Ω_0 is a discrete subset of Ω (that is, it has no limit points in Ω); (ii) f is analytic in $\Omega \setminus \Omega_0$; (iii) f has a pole (of finite order) at each point of Ω_0. See for instance [Rud87] Ch. 10.

As it turns out, the first situation of Theorem 5.7 can be excluded by the following argument. It is well-known that for all $T \in \mathcal{L}(\mathcal{H})$ with $||T|| < 1$, the inverse of $(I - T)$ exists[9]. For $z \in D = \mathbb{C}\backslash\sigma(\hat{U}_0)$, using the usual resolvent upper bound for normal operators,

$$||\mathcal{R}_0(z)\mathcal{G}|| \leq ||(\hat{\mathcal{U}}_0 - z)^{-1}\hat{\mathcal{U}}_0||\; ||\mathcal{G}|| \leq \frac{||\mathcal{G}||}{\mathrm{dist}(z, \sigma(\hat{\mathcal{U}}_0))}. \tag{5.6.19}$$

Thus the left-hand side is bounded above by 1 provided that we choose $|z| > 1 + ||\mathcal{G}||$. To see this, note that $\mathrm{dist}(z, \sigma(\hat{\mathcal{U}}_0)) = \inf_{\mu\in\sigma(\hat{\mathcal{U}}_0)} |z - \mu| \geq |z| - 1$. Consequently there always exist $z \in D$ such that $I - \mathcal{R}_0(z)\mathcal{G}$ is invertible and this rules out case 1 of Theorem 5.7.

Hence the IQW has (at least one) eigenvalue provided condition (5.6.18) of Theorem 5.6 is satisfied *in the allowed set*, i.e. there exists $e^{\mathrm{i}\omega} \in D \setminus D_0$ (here D_0 is a discrete subset of D, i.e. it does not contain limit points in D) such that $1 \in \sigma\left(A(e^{\mathrm{i}\omega})D(0)\right)$. Moreover we know that $(I - \mathcal{R}_0(z)\mathcal{G})^{-1}$ exists for all $z \in D \setminus D_0$ and it is meromorphic in D with possible poles belonging to D_0.

The previous discussion raises the following questions:

(Q1) Is $A(z) : D \setminus D_0 \to \mathcal{M}_4(\mathbb{C})$ given by Theorem (5.6.12) analytic?

(Q2) Can we give examples where condition 2 of 5.6 is cannot be satisfied, i.e. that there are not eigenvalues in the gaps?

(Q3) Is the multiplicity of 1 as an eigenvalue of $A(e^{\mathrm{i}\omega})D(0)$ equal to the multiplicity of $e^{\mathrm{i}\omega}$ as an element in $\sigma_p(\mathcal{U})$?

(Q4) Can we rule out the existence of embedded eigenvalues in the continuous spectrum?

While (Q3) and (Q4) are left as future work, in the remaining part of this subsection we answer (Q1) and (Q2).

Proposition 5.8. *Let $D = \mathbb{C} \setminus \sigma(\hat{\mathcal{U}}_0)$, and D_0 a discrete subset of D such that the operator $(I - \mathcal{R}_0(z)\mathcal{G})^{-1}$ is meromorphic in D, and that $(I - \mathcal{R}_0(z)\mathcal{G})^{-1}\hat{\psi}(k) \in C(\mathbb{T};\mathbb{C}^4)$ for all $\psi(k) \in C^\infty(\mathbb{T};\mathbb{C}^4)$. Then the matrix-valued function $A : D \setminus D_0 \to \mathcal{M}_4(\mathbb{C})$,*

$$A(z) = \frac{1}{2\pi}\int_{\mathbb{T}} (I - \mathcal{R}_0(z)\mathcal{G})^{-1} R_0(z, k)\, \mathrm{d}k \tag{5.6.20}$$

is analytic in $D \setminus D_0$.

Proof. We proceed in two steps, first proving continuity and then deriving analyticity as a consequence of Morera's theorem.

Continuity. Since $(I - \mathcal{R}_0(z)\mathcal{G})^{-1}$ is analytic in $D \setminus D_0$, and $\mathcal{R}_0(z)$ is analytic in D, then their product is analytic at $D \setminus D_0$, because analytic functions form a ring. Let $z_0 \in D \setminus D_0$, and choose $\delta_0 > 0$ such that $B(z_0, \delta_0) = \{z \in \mathbb{C} : |z - z_0| < \delta\} \subset D \setminus D_0$. For $z \in B(z_0, \delta_0)$, $(I - \mathcal{R}_0(z)\mathcal{G})^{-1}R_0(z, k)$ is continuous as a function of (z, k) and hence

[9] See for instance [GGK03] Section 2.8.

uniformly continuous on $\overline{B(z_0, \delta_0)} \times [-\pi, \pi]$. Thus, given $\varepsilon > 0$ there exists $\delta_1 > 0$ such that

$$||(I - \mathcal{R}_0(z)\mathcal{G})^{-1}R_0(z,k) - (I - \mathcal{R}_0(z_0)\mathcal{G})^{-1}R_0(z_0,k)|| < \varepsilon. \tag{5.6.21}$$

Hence for $\delta = \min\{\delta_0, \delta_1\}$, from (5.6.20) we deduce

$$||A(z) - A(z_0)|| < \varepsilon \tag{5.6.22}$$

for all $z \in B(z_0, \delta)$.

Analyticity. We apply Morera's Theorem. Given any closed piecewise C^1 curve γ in $D \setminus D_0$,

$$\int_\gamma A(z)\mathrm{d}z = \frac{1}{2\pi}\int_{-\pi}^{\pi}\left[\int_\gamma (I - \mathcal{R}_0(z)\mathcal{G})^{-1}R_0(z,k)\mathrm{d}z\right]\mathrm{d}k = 0. \tag{5.6.23}$$

Here the change in the order of integration is justified by continuity of the integrand on $\overline{\text{int}(\gamma)} \times [-\pi, \pi]$, and the analyticity of the integrand implies that the integral around γ is zero for all $k \in [-\pi, \pi]$. ☐

An interesting consequence is that the interaction at the contact point has a prominent role for the non-existence of eigenvalues, and this remark allows to answer (Q2). Consider an IQW which satisfies hypothesis **(H0)**, and that is also trace-class. Let $V(0) = I_4$ (i.e. the interaction at the contact point vanishes), and arbitarary $V(x)$ for $|x| \geq 1$. Since $D(0) = 0$, from Theorem 5.6, the IQW cannot have eigenvalues in the gaps of its continuous spectrum in all points where $(I - \mathcal{R}_0(e^{\mathrm{i}\omega})\mathcal{G}$ is invertible. In fact in the same lines we can deduce a slightly more general consequence. The key is to apply the previous reasoning to the case when $V(0)$ is taken "sufficiently" close to the identity.

Corollary 5.4. *Consider an IQW which satisfies hypothesis* **(H0)***, and that is also trace-class. Then* $e^{\mathrm{i}\omega} \in (D \setminus D_0) \cap \mathbb{S}$ *is such that* $e^{\mathrm{i}\omega} \notin \sigma_p(\mathcal{U}) \cap (\mathbb{S} \setminus \sigma_{ac}(\mathcal{U}))$ *if*

$$||D(0)|| < \frac{2\pi}{\displaystyle\int_{-\pi}^{\pi} ||(I - \mathcal{R}_0(e^{\mathrm{i}\omega})\mathcal{G})^{-1}R_0(e^{\mathrm{i}\omega}, k)||\mathrm{d}k}. \tag{5.6.24}$$

In particular, the IQW has no eigenvalues in the gaps of the continuous spectrum provided that

$$||D(0)|| < \frac{2\pi}{\displaystyle\max_{z\in(D\setminus D_0)\cap\mathbb{S}}\int_{-\pi}^{\pi} ||(I - \mathcal{R}_0(e^{\mathrm{i}\omega})\mathcal{G})^{-1}R_0(z, k)||\mathrm{d}k}. \tag{5.6.25}$$

Proof. If $r(A(z)D(0)) < 1$, where $r(\cdot)$ denotes the spectral radius, then the eigenvalues of $A(z)D(0)$ are in the open unit disk $\mathbb{D}$, and in particular 1 cannot be an eigenvalue, thus condition 2 of Theorem 5.6 cannot be satisfied. From Gelfand's formula, $r(A(z)D(0)) \leq ||A(z)D(0)||$, where $||\cdot||$ denotes any matrix norm[10] (although in the examples we choose

[10] See [HJ12], Theorem 5.6.9.

the Frobenius norm). The bounds above follow from

$$||A(z)D(0)|| \leq ||D(0)||\frac{1}{2\pi}\int_{-\pi}^{\pi}||(I-\mathcal{R}_0(z)\mathcal{G})^{-1}R_0(z,k)||\mathrm{d}k \tag{5.6.26}$$

for $z \in (D \setminus D_0) \cap \mathbb{S}$. $\square$

5.6.3 Reducing the integral equation to an algebraic system

From (5.6.5), we have formally that

$$G(k-k') = \sum_{x=1}^{\infty} 2D(x)\cos(k-k')x \tag{5.6.27a}$$

$$= \sum_{x=1}^{\infty} 2D(x)\cos kx \cos k'x + \sum_{x=1}^{\infty} 2D(x)\sin kx \sin k'x. \tag{5.6.27b}$$

In the following we restrict to the case where $(I-\mathcal{V})$ is trace class. As discussed in Remark 5.6, in this case both series appearing in (5.6.27b), seen as functions of k', converge uniformly for each fixed value of $k \in \mathbb{T}$. Using this fact we are able to integrate term by term the cosine and sine series appearing in (5.6.27b) by dominated convergence.[11]

For each $x \in \mathbb{Z}$, $D(x) \in \mathbb{C}^{4\times 4}$ is normal, because

$$[D(x), D^{\dagger}(x)] = [I_4 - V(x), I - V^{\dagger}(x)] = [V(x), V^{\dagger}(x)] = 0, \tag{5.6.30}$$

from unitarity of $V(x)$. Then from the spectral theorem for normal operators in finite-

[11] Suppose that we have a complex-valued sequence $a = \{a(x)\}_{x\in\mathbb{N}} \subset \mathbb{C}$ and we would like to integrate term by term in $\mathbb{T}$ the series $\sum_{x=1}^{\infty} a(x)\cos kx$, which we assume it converges for each value of k. Consider the sequence of functions $\{f_n(k)\}_{n\in\mathbb{N}}$ defined by the partial sums, i.e. $f_n(k) = \sum_{x=1}^{n} a(x)\cos kx$. To apply Lebesgue's dominated convergence theorem, we need to find a dominating function. In this case, assume that $a \in \ell^1(\mathbb{N})$. For $p, q \in \mathbb{R}$ such that $1 \leq p < q \leq \infty$, the inclusion $\ell^p(\mathbb{N}) \subset \ell^q(\mathbb{N})$ holds. Then a is also in $\ell^2(\mathbb{N})$, hence it converges to an $L^2(\mathbb{T})$ function by the Riesz-Fisher theorem. Moreover, since

$$|f_n(k)| \leq \sum_{x=1}^{n}|a(x)| \leq \sum_{x=1}^{\infty}|a(x)| = ||a||_1 \tag{5.6.28}$$

Then the constant function $||a||_1$ for all $k \in \mathbb{T}$ is a summable dominating function for all $n \geq 1$ allowing the interchange, i.e.

$$\int_{\mathbb{T}}\sum_{x=1}^{\infty} a(x)\cos kx \,\mathrm{d}k = \lim_{n\to\infty}\int_{\mathbb{T}}\sum_{x=1}^{n} a(x)\cos kx \,\mathrm{d}k = \sum_{x=1}^{\infty}\int_{\mathbb{T}} a(x)\cos kx \,\mathrm{d}k. \tag{5.6.29}$$

dimensional spaces, $D(x)$ allows a decomposition

$$D(x) = \sum_{j=1}^{4} d_{x,j}\phi_{x,j}\phi_{x,j}^{\dagger}, \qquad d_{x,j} = 1 - e^{\mathrm{i}\lambda_{x,j}}, \tag{5.6.31}$$

where the vectors $\{\phi_{x,j} \in \mathbb{C}^4\}_{j=1}^4$ are orthonormal and the eigenvalues are $\{d_{x,j}\}_{j=1}^4$, with $\{e^{\mathrm{i}\lambda_{x,j}}\}_{j=1}^4$ being the eigenvalues of $V(x)$. Let

$$\hat{g}_{x,j}^{e} := \sqrt{2}\phi_{x,j}\cos kx, \qquad \hat{g}_{x,j}^{o} := \sqrt{2}\phi_{x,j}\sin kx. \tag{5.6.32}$$

Lemma 5.5. *Let $\{\phi_{x,j}\}_j$ be the normalized eigenvectors of $D(x)$, and let $\hat{g}_{x,j}^e$ and $\hat{g}_{x,j}^o$ be defined as in* (5.6.32). *Set the multi-index $\vec{m} = (s, x, j)$, for $s \in \{e, o\}$, $x \in \mathbb{N}_0$, and $j \in \{1, \ldots, 4\}$. Then the set $\{\hat{g}_{\vec{m}}\}_{\vec{m}=(s,x,j)}$ forms an orthonormal system in $\hat{\mathcal{H}}_{rel.}$, i.e. the relation*

$$\langle \hat{g}_{\vec{m}}, \hat{g}_{\vec{m}'} \rangle = \delta_{\vec{m},\vec{m}'} \tag{5.6.33}$$

holds.

Proof. Equation (5.6.33) is equivalent to

$$\langle \hat{g}_{x_1,j_1}^e, \hat{g}_{x_2,j_2}^e \rangle = \delta_{j_1,j_2}\delta_{x_1,x_2}, \tag{5.6.34a}$$

$$\langle \hat{g}_{x_1,j_1}^o, \hat{g}_{x_2,j_2}^o \rangle = \delta_{j_1,j_2}\delta_{x_1,x_2}, \tag{5.6.34b}$$

$$\langle \hat{g}_{x,j}^e, \hat{g}_{x',j'}^o \rangle = 0. \tag{5.6.34c}$$

Beginning with the first equation, we compute

$$\begin{aligned}
\langle \hat{g}_{x_1,j_1}^e, \hat{g}_{x_2,j_2}^e \rangle &= \frac{1}{2\pi}\int_{-\pi}^{\pi} \hat{g}_{x_1,j_1}^{e\,\dagger}\hat{g}_{x_2,j_1}^e \mathrm{d}k \\
&= \frac{1}{2\pi}\int_{-\pi}^{\pi} 2\phi_{x_1,j_1}^{\dagger}\phi_{x_2,j_2}\cos kx_1 \cos kx_2 \,\mathrm{d}k \\
&= \phi_{x_1,j_1}^{\dagger}\phi_{x_2,j_2}\frac{1}{\pi}\int_{-\pi}^{\pi} \frac{\cos k(x_1 - x_2) + \cos k(x_1 + x_2)}{2}\mathrm{d}k \\
&= \delta_{j_1,j_2}\delta_{x_1,x_2}.
\end{aligned}$$

For the other cases it follows in a similar way, applying the rules of products of trigonometric functions that can be found in many places, for instance see Chapter 1 of [Tol62]. $\square$

We now substitute (5.6.27b) into (5.6.7), which leads to

$$
\begin{aligned}
(\mathcal{G}\hat{\psi})(k) =& \frac{1}{2\pi}\int_{-\pi}^{\pi} G(k-k')\hat{\psi}(k')\mathrm{d}k' \\
&= \frac{1}{2\pi}\int_{-\pi}^{\pi}\left[\sum_{x=1}^{\infty} 2D(x)\cos kx\cos k'x + \sum_{x=1}^{\infty} 2D(x)\sin kx\sin k'x\right]\hat{\psi}(k')\mathrm{d}k' \\
&= \sum_{x=1}^{\infty} 2D(x)\cos kx\left[\frac{1}{2\pi}\int_{-\pi}^{\pi}\cos k'x\;\hat{\psi}(k')\mathrm{d}k'\right] \\
&\quad + \sum_{x=1}^{\infty} 2D(x)\sin kx\left[\frac{1}{2\pi}\int_{-\pi}^{\pi}\sin k'x\;\hat{\psi}(k')\mathrm{d}k'\right] \\
&= \sum_{x,j} d_{x,j}\sqrt{2}\phi_{x,j}\cos kx\left[\frac{1}{2\pi}\int_{-\pi}^{\pi}\sqrt{2}\phi_{x,j}^{\dagger}\cos k'x\;\;\hat{\psi}(k')\mathrm{d}k'\right] \\
&\quad + \sum_{x,j} d_{x,j}\sqrt{2}\phi_{x,j}\sin kx\left[\frac{1}{2\pi}\int_{-\pi}^{\pi}\sqrt{2}\phi_{x,j}^{\dagger}\sin k'x\;\;\hat{\psi}(k')\mathrm{d}k'\right].
\end{aligned}
$$

The last equation was arranged so that we recognise an inner product. We arrive at

$$
(\mathcal{G}\hat{\psi})(k) = \sum_{x=1}^{\infty}\sum_{j=1}^{4} d_{x,j}\left(\langle\hat{g}_{x,j}^{e},\hat{\psi}\rangle\hat{g}_{x,j}^{e}(k) + \langle\hat{g}_{x,j}^{o},\hat{\psi}\rangle\hat{g}_{x,j}^{o}(k)\right). \tag{5.6.35}
$$

Expression (5.6.35) is the canonical decomposition of a compact operator. It is clear that the spectral decomposition of the integral operator $\mathcal{G}$ can be given explicitly once that of $V(x)$ is known,

$$
\sigma(\mathcal{G}) = \{0\} \cup \{d_{x,j} : x \in \mathbb{N}, 1 \leq j \leq 4 \text{ (with double multiplicity)}\}. \tag{5.6.36}
$$

Plugging (5.6.35) into the eigenvalue equation (5.6.9), we arrive at

$$
D(0)N_0\hat{\psi} + \sum_{x,j}\sum_{s} d_{x,j}\langle\hat{g}_{x,j}^{s},\hat{\psi}\rangle\hat{g}_{x,j}^{s} = \hat{U}_0^{-1}(\hat{U}_0 - e^{\mathrm{i}\omega})\hat{\psi}. \tag{5.6.37}
$$

The index s refers to the parity of the eigenvectors, either e (even) or o (odd). Note that the leftmost term is a "source" term, $D(0)N_0\hat{\psi} = D(0)\psi(0)$, independent of k. However it is not an independent term, since the solution of the equation is linked to it via $\psi(0)$: it is rather a *compatibility* condition which specifies that solutions $\hat{\psi}$ of (5.6.9) must satisfy Eq. (5.6.6).

To conclude, we project (5.6.37) into the basis $\{\hat{g}_{\vec{m}}\}_{\vec{m}}$, reducing the problem to a (possibly infinite) system of algebraic equations in the coefficients $\langle\hat{g}_{\vec{m}},\hat{\psi}\rangle$. Multiplying (5.6.37) from the left by $\mathcal{R}_0$, we arrive at

$$
\mathcal{R}_0(e^{\mathrm{i}\omega})D(0)N_0\hat{\psi} + \sum_{\vec{m}:\, x\geq 1} d_{x,j}\langle\hat{g}_{\vec{m}},\hat{\psi}\rangle\mathcal{R}_0(e^{\mathrm{i}\omega})\hat{g}_{\vec{m}} = \hat{\psi}. \tag{5.6.38}
$$

We summarize the content of this section in the following theorem.

Theorem 5.8. *Consider the eigenvalue problem for $\hat{\mathcal{U}}$ as in* (5.6.1)-(5.6.2). *Assume that **(H0)** holds, and additionally that $(I-\mathcal{V}) \in \mathfrak{S}_1$. Let $e^{\mathrm{i}\omega} \notin \sigma(\hat{\mathcal{U}}_0)$ for some $\omega \in \mathbb{T}$. Then, $e^{\mathrm{i}\omega}$ is an eigenvalue of $\hat{\mathcal{U}}$ with associated eigenvector $\hat{\psi} \in \hat{\mathcal{H}}_{rel.}$ if and only if $\hat{\psi}$ is a non-trivial solution of Eq.* (5.6.38) *for the same value of ω.*

A system of equations as that given by (5.6.38), is typically solved by projecting on the basis elements.

Finite range interactions. Rank N interactions are translated into the following system of equations. Let $d_{x,j}$ be zero for $x \geq N$. Projecting Eq. (5.6.38) into $\hat{g}^{s'}_{x',j'}$, with $s' = e, o$, we find

$$\langle \hat{g}^{s'}_{x',j'}, R_0 D(0) N_0 \hat{\psi} \rangle + \sum_{x=1}^{N} \sum_{j=1}^{4} \sum_{s=e,o} d_{x,j} \langle \hat{g}^{s}_{x,j}, \hat{\psi} \rangle \langle \hat{g}^{s'}_{x',j'}, R_0 \hat{g}^{s}_{x,j} \rangle = \langle \hat{g}^{s'}_{x',j'}, \hat{\psi} \rangle. \tag{5.6.39}$$

Infinite range interactions. Infinite range interactions are translated into the following system of equations. Projecting Eq. (5.6.38) into $\hat{g}^{s'}_{x',j'}$,

$$\langle \hat{g}^{s'}_{x',j'}, R_0 \varphi_0 \rangle + \sum_{x=1}^{\infty} \sum_{j=1}^{4} \sum_{s=e,o} d_{x,j} \langle \hat{g}^{s}_{x,j}, \hat{\psi} \rangle \langle \hat{g}^{s'}_{x',j'}, R_0 \hat{g}^{s}_{x,j} \rangle = \langle \hat{g}^{s'}_{x',j'}, \hat{\psi} \rangle. \tag{5.6.40}$$

5.6.3.1 Further properties of $\mathcal{R}_0(e^{\mathrm{i}\omega})$

We denote by $\{E_0(\cdot)\}$ the spectral family associated to $\hat{\mathcal{U}}_0$, i.e.

$$\langle \hat{\psi}, \hat{\mathcal{U}}_0^n \hat{\psi} \rangle = \int_{\mathbb{T}} e^{\mathrm{i}n\theta} \mathrm{d} \langle \hat{\psi}, E_0(\theta) \hat{\psi} \rangle = \int_{\mathbb{T}} e^{\mathrm{i}n\theta} d\mu_{\hat{\psi}}(\theta), \tag{5.6.41}$$

for all $\hat{\psi} \in \hat{\mathcal{H}}_{rel.}$ and $n \in \mathbb{Z}$. Let $r \neq 1$ and $\theta \in \mathbb{T}$, then

$$\mathcal{R}_0(re^{\mathrm{i}\theta}) = (\hat{\mathcal{U}}_0 - re^{\mathrm{i}\theta})^{-1} \hat{\mathcal{U}}_0 = (I - re^{\mathrm{i}\theta} \hat{\mathcal{U}}_0^*)^{-1}, \tag{5.6.42}$$

and we let

$$2\pi \delta_r(E_0, \theta) = \mathcal{R}_0(re^{\mathrm{i}\theta}) - \mathcal{R}_0(r^{-1} e^{\mathrm{i}\theta}). \tag{5.6.43}$$

Lemma 5.6. *(see [KK70]) For any pair of vectors $\hat{\psi}, \hat{\phi} \in \hat{\mathcal{H}}_2$,*

$$\lim_{r \to 1^-} \langle \hat{\psi}, \delta_r(E_0, \theta) \hat{\phi} \rangle = \frac{d}{d\theta} \langle \hat{\psi}, E_{0,a.c.}(\theta) \hat{\phi} \rangle, \qquad a.e. \;\; \theta \in \mathbb{T} \tag{5.6.44}$$

where $E_{0,a.c.}(\theta)$ is the absolutely continuous part of the spectral projector of $\hat{U}_0$ at $e^{\mathrm{i}\theta}$.

The following result which we adapt to our context, appears in [AC11]. It assumes that $\hat{\mathcal{U}}_0$ is purely absolutely continuous, which always holds in the IQW.

Theorem 5.9. *(see [AC11]) Consider an IQW satisfying* **(H0)**. *Assume that such that for some $e^{\mathrm{i}\omega} \in \mathbb{T}$ and some $\hat{g}_{\vec{m}'}$, the limit*

$$\hat{v}_{\vec{m}'} := \lim_{r \to 1^-} (\hat{U}_0 - re^{\mathrm{i}\omega})^{-1} \hat{U}_0 \hat{g}_{\vec{m}'} \tag{5.6.45}$$

exists. Then,

$$\langle \hat{g}_{\vec{m}}, \hat{v}_{\vec{m}'} \rangle = \frac{1}{2} \delta_{\vec{m},\vec{m}'} + \frac{\mathrm{i}}{2} \int_{\mathbb{S}} \cot\left(\frac{\omega - \theta}{2}\right) \mathrm{d}\langle \hat{g}_{\vec{m}}, E_0(\theta) \hat{g}_{\vec{m}'} \rangle. \tag{5.6.46}$$

Moreover,

$$\langle \hat{g}_{\vec{m}}, \hat{v}_{\vec{m}'} \rangle = -\overline{\langle \hat{g}_{\vec{m}'}, \hat{v}_{\vec{m}} \rangle}. \tag{5.6.47}$$

Let us note that the limit (5.6.45) always exists if we choose $e^{\mathrm{i}\omega} \notin \sigma(\hat{\mathcal{U}}_0)$. Thus, formulas (5.6.46)-(5.6.47) are another way of writing the coefficients appearing in the algebraic system (5.6.40).

Suppose otherwise that $e^{\mathrm{i}\omega} \in \sigma(\mathcal{U}_0)$, that is, it is embedded in the continuous spectrum, and we ask if the limit (5.6.45) exists. Without giving a complete answer to the question, below we reformulate it in terms of the eigenvectors of the free QW, that were computer explicitly (see 5.3.3.2). Consider the spectral decomposition of $\hat{U}_0(k)$,

$$\hat{U}_0(k) = \sum_{\ell=1,2} e^{\mathrm{i}\lambda_{\ell,+}} |u_{\ell,+}\rangle\langle u_{\ell,+}| + e^{\mathrm{i}\lambda_{\ell,-}} |u_{\ell,-}\rangle\langle u_{\ell,-}|. \tag{5.6.48}$$

Then, for $r < 1$,

$$(\hat{U}_0(k) - re^{\mathrm{i}\omega})^{-1} = \sum_{\ell=1,2} \frac{1}{e^{\mathrm{i}\lambda_{\ell,+}} - re^{\mathrm{i}\omega}} |u_{\ell,+}\rangle\langle u_{\ell,+}| + \frac{1}{e^{\mathrm{i}\lambda_{\ell,-}} - re^{\mathrm{i}\omega}} |u_{\ell,-}\rangle\langle u_{\ell,-}|, \tag{5.6.49}$$

and consequently

$$\begin{aligned} \hat{v}_{\vec{m}} &= \lim_{r \to 1^-} (\hat{U}_0 - re^{\mathrm{i}\omega})^{-1} \hat{U}_0 \hat{g}_{\vec{m}} \\ &= \lim_{r \to 1^-} \sum_{\ell=1,2} \frac{e^{\mathrm{i}\lambda_{\ell,+}}}{e^{\mathrm{i}\lambda_{\ell,+}} - re^{\mathrm{i}\omega}} |u_{\ell,+}\rangle\langle u_{\ell,+}, \hat{g}_{\vec{m}}\rangle + \frac{e^{\mathrm{i}\lambda_{\ell,-}}}{e^{\mathrm{i}\lambda_{\ell,-}} - re^{\mathrm{i}\omega}} |u_{\ell,-}\rangle\langle u_{\ell,-}, \hat{g}_{\vec{m}}\rangle. \end{aligned} \tag{5.6.50}$$

Integrals of the form

$$c_{\ell,\pm,s}(x) := \langle u_{\ell,\pm}, \hat{g}_{\vec{m}} \rangle = \frac{1}{\sqrt{2\pi}} \int_{-\pi}^{\pi} u^\dagger_{\ell,\pm}(k) \cdot \phi_{x,j} \left\{ \begin{array}{c} \cos kx \\ \sin kx \end{array} \right\} \mathrm{d}k \tag{5.6.51}$$

can in general be evaluated via residues, and the result is a function of x only (not of k). Suppose that there is $k \in \mathbb{T}$ such that, say, $\lambda_{1,+}(k) = \omega \mod 2\pi$. Then we have a divergence, i.e. $e^{\mathrm{i}\lambda_{1,+}} - re^{\mathrm{i}\omega} \to 0$ when $r \to 1^-$. For the limit to exist we require that

$\hat{v}_{\vec{m}} \in L^2(\mathbb{T}, \mathbb{C}^4)$, and in turn this implies that limits of the form

$$\lim_{r \to 1^-} \frac{\langle u_{1,+}, u_{1,+} \rangle}{|e^{\mathrm{i}\lambda_{1,+}} - re^{\mathrm{i}\omega}|^2} \tag{5.6.52}$$

exist. The existence of this kind of limit can be explored with the help of the formulae for the eigenvectors obtained in Subsection 5.3.3.2.

To conclude this section, let us take a closer look at the object $\langle \hat{g}^{s'}_{x',j'}, R_0(e^{\mathrm{i}\omega})\hat{g}^{s}_{x,j} \rangle$. We can exploit the property that $\hat{U}_0(k)$ depends on k in a simple way, namely that rows 2 and 3 are multiplied by $e^{-2\mathrm{i}k}$ and $e^{2\mathrm{i}k}$ respectively, the other rows being independent of k (see Proposition 5.2). Let us write $(\hat{U}_0(k) - e^{\mathrm{i}\omega})^{-1} = d_0(e^{\mathrm{i}\omega})^{-1}\mathrm{cof}(\hat{U}_0(k) - e^{\mathrm{i}\omega})^{\mathsf{T}}$, where $\mathrm{cof}(\cdot)$ is the cofactor matrix, and $d_0(e^{\mathrm{i}\omega}) = \det(\hat{U}_0(k) - e^{\mathrm{i}\omega})$. Seen now as functions of $k \in \mathbb{T}$ with fixed $e^{\mathrm{i}\omega}$, and setting $\mu = e^{2\mathrm{i}k}$, both d_0 and the matrix elements of the cofactor matrix are polynomials in μ, μ^{-1} of order 1. Then, the matrix elements of $R_0(e^{\mathrm{i}\omega}, k) = (\hat{U}_0(k) - e^{\mathrm{i}\omega})^{-1}\hat{U}_0(k)$ are rational functions on μ of order 4, more precisely,

$$[R_0(e^{\mathrm{i}\omega}, \mu)]_{ij} = \frac{\sum_{\ell=-2}^{2} \alpha_\ell^{ij} \mu^\ell}{\sum_{\ell=-1}^{1} \beta_\ell^{ij} \mu^\ell}, \qquad \mu = e^{2\mathrm{i}k}. \tag{5.6.53}$$

Then

$$\begin{aligned} \langle \hat{g}^{s'}_{x',j'}, R_0(e^{\mathrm{i}\omega})\hat{g}^{s}_{x,j} \rangle &= 2\phi^{\dagger}_{x,j} \left[\frac{1}{2\pi} \int_{-\pi}^{\pi} \left\{ \begin{array}{c} \cos kx' \\ \sin kx' \end{array} \right\} R_0(e^{\mathrm{i}\omega}, k) \left\{ \begin{array}{c} \cos kx \\ \sin kx \end{array} \right\} \mathrm{d}k \right] \phi_{x,j} \\ &= 2\phi^{\dagger}_{x,j} Q(x, x', s, s')\phi_{x,j}. \end{aligned} \tag{5.6.54}$$

The integral in brackets, $Q(x, x', s, s') \in \mathcal{M}_4(\mathbb{C})$, can in general be evaluated via complex analysis using (5.6.53) (for instance first computing the zeros of d_0, developing in simple fractions and applying Cauchy's residue theorem[12]). Component-wise we have af-

[12] Recall that the computation of a trigonometric integral of the form $\frac{1}{2\pi}\int_{-\pi}^{\pi} Q(\cos k, \sin k)\mathrm{d}k$, where Q is a rational function of two variables, which we assume is continuous on $\mathbb{S} = \partial\mathbb{D}$, can be reduced to pole evaluation inside the unit circle via Cauchy's residue theorem. Recall that if z_i is a pole of order n, then

$$\mathrm{Res}(f, z_i) = \frac{1}{(n-1)!} \lim_{z \to z_i} \frac{d^{n-1}}{dz^{n-1}} \left((z - z_i)^n f(z) \right). \tag{5.6.55}$$

If we let $f(z) = \dfrac{Q\left(\frac{1}{2}\left(z + \frac{1}{z}\right), \frac{1}{2\mathrm{i}}\left(z - \frac{1}{z}\right)\right)}{\mathrm{i}z}$, then the following formula holds:

$$\frac{1}{2\pi} \int_{-\pi}^{\pi} Q(\cos k, \sin k)\, \mathrm{d}k = \mathrm{i} \sum_{z_i \in \mathbb{D}} \mathrm{Res}(f, z_i). \tag{5.6.56}$$

ter the change of variables $\mu = e^{2\mathrm{i}k}$ and some elementary manipulations, that

$$[Q(x,x',s,s')]_{ij} = -\frac{\mathrm{i}}{16\pi}\oint_{\mathbb{S}'}[R_0(e^{\mathrm{i}\omega},\mu)]_{ij}\,\mu^{-\frac{x'}{2}-\frac{x}{2}-1}\left\{\begin{array}{c}1+\mu^{x'}\\ \mathrm{i}-\mathrm{i}\mu^{-x'}\end{array}\right\}\left\{\begin{array}{c}1+\mu^{x}\\ \mathrm{i}-\mathrm{i}\mu^{-x}\end{array}\right\}\mathrm{d}\mu. \tag{5.6.57}$$

Where $\mathbb{S}' = \{z \in \mathbb{C} : z = e^{2\mathrm{i}k}, k \in \mathbb{T}\}$ denotes two loops around the unit circle $\mathbb{S}$.

5.7 Examples

5.7.1 Contact interaction revisited

The case of an IQW with contact (or point) interaction is defined by

$$V(x) = V_0\delta_{x,0} + (1-\delta_{x,0})I_4, \qquad x \in \mathbb{Z}, \tag{5.7.1}$$

where $\delta_{x,0}$ is a Kronecker delta and $V_0 \in U(4)$, with eigenvalues $\{e^{\mathrm{i}\lambda_j}\}_{j=1}^4$.

The contact interaction was studied in [AAM+12], in particular with the free QW given by the Hadamard walk and $V_0 = e^{\mathrm{i}g}I_4$. In this setting, the authors found that $\mathcal{U}$ admits eigenvalues that lie in the gaps of the continuous spectrum, and for a fixed initial condition $\psi(0) = \psi_- = (0,1,-1,0)^{\mathsf{T}}/\sqrt{2}$, the position of the eigenvalues over $\mathbb{S}$ was obtained analytically. They also proved that allowing general $V(0) \in U(4)$, the inverse problem can always be solved.

In this section we revisit the problem of contact interactions. In addition of presenting some intermediate steps and details not included in [AAM+12], we contribute in several directions:

(1) We compute in full $R_0(e^{\mathrm{i}\omega},k)$ and $A(e^{\mathrm{i}\omega})$. We remark that these expressions are useful because (i) with them one can analyse arbitrary initial conditions; (ii) they prepare the ground for studying more complicated IQW problems (e.g. non-contact interactions) in which the free walk is given by the Hadamard walk.

(2) We study and give conditions for the *direct* problem, that is, the existence of eigenvalues for a given $V_0 \in U(4)$.

5.7.1.1 Spectrum of $\hat{\mathcal{U}}_0$ and gap condition

We fix the free walk to be given by Hadamard walks, that is, we set once and for all $C_1 = C_2 = H$ (see (5.3.13) of Example 5.3.1). Then, from Proposition 5.2,

$$\hat{U}_0(k) = \frac{1}{2}\begin{pmatrix} e^{-\mathrm{i}p} & e^{-\mathrm{i}p} & e^{-\mathrm{i}p} & e^{-\mathrm{i}p}\\ e^{-2\mathrm{i}k} & -e^{-2\mathrm{i}k} & e^{-2\mathrm{i}k} & -e^{-2\mathrm{i}k}\\ e^{2\mathrm{i}k} & e^{2\mathrm{i}k} & -e^{2\mathrm{i}k} & -e^{2\mathrm{i}k}\\ e^{\mathrm{i}p} & -e^{\mathrm{i}p} & -e^{\mathrm{i}p} & e^{\mathrm{i}p}\end{pmatrix}. \tag{5.7.2}$$

Let us consider the band structure of the spectrum. It follows from Remark 5.5 that the critical values of $\lambda_{1,\pm}(k)$ are $\{0, \pm\pi\}$, and those of $\lambda_{2,\pm}(k)$ are $\{\pm\pi/2\}$. The evaluation of $\lambda_{1,\pm}(k)$ and $\lambda_{2,\pm}(k)$ at these special points is straightforward from (5.3.19); the result appears in Table 5.7.1.

	$\lambda_{1,+}(k)$	$\lambda_{1,-}(k)$	$\lambda_{2,+}(k)$	$\lambda_{2,-}(k)$
$k=0$	$-e^{2\mathrm{i}\arccos\left(\frac{1}{\sqrt{2}}\sin p/2\right)}$	$-e^{-2\mathrm{i}\arccos\left(\frac{1}{\sqrt{2}}\sin p/2\right)}$	-1	-1
$k=\pm\pi$	$-e^{-2\mathrm{i}\arccos\left(\frac{1}{\sqrt{2}}\sin p/2\right)}$	$-e^{2\mathrm{i}\arccos\left(\frac{1}{\sqrt{2}}\sin p/2\right)}$	-1	-1
$k=\pi/2$	1	1	$e^{2\mathrm{i}\arccos\left(\frac{1}{\sqrt{2}}\cos p/2\right)}$	$e^{-2\mathrm{i}\arccos\left(\frac{1}{\sqrt{2}}\cos p/2\right)}$
$k=-\pi/2$	1	1	$e^{-2\mathrm{i}\arccos\left(\frac{1}{\sqrt{2}}\cos p/2\right)}$	$e^{2\mathrm{i}\arccos\left(\frac{1}{\sqrt{2}}\cos p/2\right)}$

Table 5.7.1: Evaluation of $\lambda_{1,\pm}(k)$ and $\lambda_{2,\pm}(k)$ for the Hadamard walk at critical points.

5.7.1.2 Eigenvalue problem

Since (5.7.1) implies that $d_{x,j} = 0$ for $x \geq 1$, then the only surviving term is the source term, because $\mathcal{G}$ is identically zero, and the eigenvalue equation (cf. (5.6.9)) is $\mathcal{R}_0(e^{\mathrm{i}\omega})D(0)N_0\hat{\psi} = \hat{\psi}$. In terms of the notation introduced in Subsection (5.6.2), $F(z) = (I - \mathcal{R}_0(z)\mathcal{G})^{-1} = I$ and consequently

$$A(e^{\mathrm{i}\omega}) = \frac{1}{2\pi}\int_{-\pi}^{\pi} R_0(e^{\mathrm{i}\omega})\mathrm{d}k, \qquad e^{\mathrm{i}\omega} \notin \sigma(\mathcal{U}_0). \tag{5.7.3}$$

Theorem (5.6) gives a first characterization of the eigenvalue problem. Clearly for contact interactions, both **(H0)** and trace-class conditions are trivially satisfied.

Lemma 5.7. *Consider an IQW with a contact interaction, $D(x) = \delta_{x,0}(I_4 - V_0)$ with $V_0 \in U(4)$. Then,*

$$e^{\mathrm{i}\omega} \in \sigma_p(\mathcal{U}) \iff 1 \in \sigma\left(A(e^{\mathrm{i}\omega})D(0)\right). \tag{5.7.4}$$

The following characterization of $A(e^{\mathrm{i}\omega})$ is a restatement of a result which appears in [AAM+12].

Lemma 5.8. *For $e^{\mathrm{i}\omega} \notin \sigma(\mathcal{U}_0)$, the matrix*

$$I_4 - A(e^{\mathrm{i}\omega})^{-1} \tag{5.7.5}$$

is unitary, and

$$A(e^{\mathrm{i}\omega}) = \frac{I_4}{2} + \frac{\mathrm{i}H(e^{\mathrm{i}\omega})}{2}, \tag{5.7.6}$$

with H self-adjoint.

Combining Lemma 5.7 with Lemma 5.8, we get a refined condition.

Theorem 5.10. *Consider an IQW with a contact interaction, $D(x) = \delta_{x,0}(I_4 - V_0)$, and let $V_0 = e^{\mathrm{i}g} I_4$ for some $g \in [-\pi, \pi) \setminus \{0\}$. Then, counting multiplicities,*

$$e^{\mathrm{i}\omega} \in \sigma_p(\mathcal{U}) \iff \frac{\sin g}{1 - \cos g} \in \sigma\left(H(e^{\mathrm{i}\omega})\right). \tag{5.7.7}$$

Proof. Let $c = 1 - e^{\mathrm{i}g}$. From Lemma 5.7, we deduce that

$$\begin{aligned} e^{\mathrm{i}\omega} \in \sigma_p(\mathcal{U}) &\iff 1 \in \sigma\left(AD(0)\right) && \text{(5.7.8a)} \\ &\iff 1 \in \sigma\left(cA\right) && \text{(5.7.8b)} \\ &\iff 1/c \in \sigma\left(A\right) && \text{(5.7.8c)} \\ &\iff \frac{1}{2} + \frac{\mathrm{i}}{2}\frac{\sin g}{1 - \cos g} \in \sigma\left(A\right), && \text{(5.7.8d)} \end{aligned}$$

in the last equation we used the formula

$$\frac{1}{c} = \frac{1}{1 - e^{\mathrm{i}g}} = \frac{1}{2} + \frac{\mathrm{i}}{2}\frac{\sin g}{1 - \cos g}. \tag{5.7.9}$$

By Lemma 5.8, we find that

$$e^{\mathrm{i}\omega} \in \sigma_p(\mathcal{U}) \iff \frac{1}{2} + \frac{\mathrm{i}}{2}\frac{\sin g}{1 - \cos g} \in \sigma\left(\frac{I_4}{2} + \frac{\mathrm{i}}{2}H\right). \tag{5.7.10}$$

By spectral mapping, this implies

$$\frac{\sin g}{1 - \cos g} \in \sigma(H(e^{\mathrm{i}\omega})). \tag{5.7.11}$$

□

In particular, the previous result solves the inverse problem. Suppose that we fix the position of an eigenvalue $e^{\mathrm{i}\omega} \in \mathbb{S} \setminus \sigma(\hat{U}_0)$ and compute the eigenvalues of $H(e^{\mathrm{i}\omega})$ (four, counting multiplicities), which will be real because it is an hermitian matrix. Then since $\operatorname{Im} \frac{\sin g}{1-\cos g} = \mathbb{R} \setminus \{0\}$, there is always $g \in [-\pi, \pi) \setminus \{0\}$ such that condition (5.7.11) is satisfied.

5.7.1.3 Evaluation of $R_0(e^{\mathrm{i}\omega}, k)$

Next we compute $R_0(e^{\mathrm{i}\omega}, k) = (\hat{U}_0(k) - e^{\mathrm{i}\omega})^{-1}\hat{U}_0(k)$. The inverse was taken symbolically with the package `sagemath`[13]. Let

$$[R_0(e^{\mathrm{i}\omega}, \mu)]_{ij} = \frac{\alpha_2^{ij}\mu^2 + \alpha_1^{ij}\mu + \alpha_0^{ij}}{\beta_2\mu^2 + \beta_1\mu + \beta_0}, \quad \mu = e^{2\mathrm{i}k}, \tag{5.7.12}$$

[13] Some useful references are `http://www.sagemath.org/` and `http://ask.sagemath.org`. Also the book [CCC+13] is an excellent introduction.

$i, j = 1, \ldots, 3$. Comparing to the general rational expression (5.6.53), we see that the Hadamard case is already simpler in the sense that it is of order 2 in μ, instead of being of order 4.

The determinant is $d_0(\mu) = \beta_2\mu^2 + \beta_1\mu + \beta_0$ with

$$\beta_2 = \beta_0 = \cos\omega - \cos p \tag{5.7.13a}$$

$$\beta_1 = 2\left(\cos 2\omega - \cos\omega\cos p\right). \tag{5.7.13b}$$

For the sequel, we are interested in the roots of $d_0(\mu)$ and its position with respect to the unit circle.

1. If $\cos\omega = \cos p$, then $d_0(\mu) = \beta\mu$ with $\beta = -2\sin^2\omega$. Then $d_0(\mu) = 0$ if and only if $\mu\sin^2\omega = 0$, so that $\mathcal{Z}(d_0) = \{\mu_1 = 0\}$ if $\omega \notin \{-\pi, 0, \pi\}$ and otherwise it is the constant null function.

2. If $\cos\omega \neq \cos p$, then $d_0(\mu) = \beta(\mu - \mu_1)(\mu - \mu_2)$, with $\beta = \cos\omega - \cos p$, $\beta \neq 0$. Then

   $$d_0(\mu) = 0 \iff \mu^2 + 2\mu f(\omega, p) + 1 = 0, \tag{5.7.14}$$

   where

   $$f(\omega, p) = \frac{\cos 2\omega - \cos\omega\cos p}{\cos\omega - \cos p}. \tag{5.7.15}$$

   Then $\mathcal{Z}(d_0) = \{\mu_1 = -f + \sqrt{f^2 - 1}, \mu_2 = -f - \sqrt{f^2 - 1}\}$. We have two subcases:

   (a) If $|f(\omega, p)| \leq 1$, then the roots are one complex conjugate of the other and are located over $\mathbb{S}$. In particular $\mu_1, \mu_2 \notin \mathbb{D}$.

   (b) If $|f(\omega, p)| > 1$, then there are two distinct real roots. In particular:

   (b.i) If $f > 1$ then $\mu_1 \in \mathbb{D}$ and $\mu_2 \notin \mathbb{D}$.

   (b.ii) If $f < -1$, then $\mu_1 \notin \mathbb{D}$ and $\mu_2 \in \mathbb{D}$.

The region of $(\omega, p) \in \mathbb{T}^2$ corresponding to each case are outlined below. Let $u = \cos\omega - \cos p$. Then

if

- $u > 0$
  - $u \geq \dfrac{\sin^2\omega}{1 + \cos\omega}$ — $-1 \leq f < 1$
  - $u < \dfrac{\sin^2\omega}{1 + \cos\omega}$ — $f < -1$
- $u < 0$
  - $u > -\dfrac{\sin^2\omega}{1 - \cos\omega}$ — $f > 1$
  - $u \leq -\dfrac{\sin^2\omega}{1 - \cos\omega}$ — $-1 < f \leq 1$

The coefficients of $R_0(e^{\mathrm{i}\omega}, k)$, sorted by order in μ, are presented in Table 5.7.2. Only the coefficients of the numerators are shown, since the denominator is common, cf. (5.7.12).

Coefficient	**Matrix element**			
	$[R_0]_{11}$	$[R_0]_{12}$	$[R_0]_{13}$	$[R_0]_{14}$
α_2^{ij}	$\frac{1}{2}(e^{-\mathrm{i}\omega} - e^{-\mathrm{i}p})$	$\frac{1}{2}(e^{-\mathrm{i}\omega} - e^{-\mathrm{i}p})$	0	0
α_1^{ij}	$e^{-2\mathrm{i}\omega} - e^{-\mathrm{i}p}\cos\omega$	$\frac{1}{2}(-e^{\mathrm{i}\omega-\mathrm{i}p} + 1)$	$\frac{1}{2}(-e^{\mathrm{i}\omega-\mathrm{i}p} + 1)$	$-\mathrm{i}e^{-\mathrm{i}p}\sin\omega$
α_0^{ij}	$\frac{1}{2}(e^{-\mathrm{i}\omega} - e^{-\mathrm{i}p})$	0	$\frac{1}{2}(e^{-\mathrm{i}\omega} - e^{-\mathrm{i}p})$	0
	$[R_0]_{21}$	$[R_0]_{22}$	$[R_0]_{23}$	$[R_0]_{24}$
α_2^{ij}	0	0	0	0
α_1^{ij}	$\frac{1}{2}(e^{-\mathrm{i}\omega+\mathrm{i}p} - 1)$	$e^{-2\mathrm{i}\omega} - e^{-\mathrm{i}\omega}\cos p$	0	$\frac{1}{2}(-e^{-\mathrm{i}\omega-\mathrm{i}p} + 1)$
α_0^{ij}	$\frac{1}{2}(-e^{\mathrm{i}\omega} + e^{\mathrm{i}p})$	$\cos\omega - \cos p$	$-\mathrm{i}\sin\omega$	$\frac{1}{2}(e^{\mathrm{i}\omega} - e^{-\mathrm{i}p})$
	$[R_0]_{31}$	$[R_0]_{32}$	$[R_0]_{33}$	$[R_0]_{34}$
α_2^{ij}	$\frac{1}{2}(-e^{\mathrm{i}\omega} + e^{\mathrm{i}p})$	$-\mathrm{i}\sin\omega$	$\cos\omega - \cos p$	$\frac{1}{2}(e^{\mathrm{i}\omega} - e^{-\mathrm{i}p})$
α_1^{ij}	$\frac{1}{2}(e^{-\mathrm{i}\omega+\mathrm{i}p} - 1)$	0	$e^{-2\mathrm{i}\omega} - e^{-\mathrm{i}\omega}\cos p$	$\frac{1}{2}(-e^{-\mathrm{i}\omega-\mathrm{i}p} + 1)$
α_0^{ij}	0	0	0	0
	$[R_0]_{41}$	$[R_0]_{42}$	$[R_0]_{43}$	$[R_0]_{44}$
α_2^{ij}	0	$\frac{1}{2}(e^{\mathrm{i}p} - e^{-\mathrm{i}\omega})$	0	$\frac{1}{2}(e^{-\mathrm{i}\omega} - e^{\mathrm{i}p})$
α_1^{ij}	$-\mathrm{i}e^{\mathrm{i}p}\sin\omega$	$\frac{1}{2}(e^{\mathrm{i}\omega+\mathrm{i}p} - 1)$	$\frac{1}{2}(e^{\mathrm{i}\omega+\mathrm{i}p} - 1)$	$e^{-2\mathrm{i}\omega} - e^{\mathrm{i}p}\cos\omega$
α_0^{ij}	0	0	$\frac{1}{2}(-e^{-\mathrm{i}\omega} + e^{\mathrm{i}p})$	$\frac{1}{2}(e^{-\mathrm{i}\omega} - e^{\mathrm{i}p})$

Table 5.7.2: Evaluation of $R_0(e^{\mathrm{i}\omega}, k)$.

5.7.1.4 Evaluation of $A(e^{\mathrm{i}\omega})$ and its spectrum

Using the generic expression (5.7.12) into (5.7.3), we deduce

$$[A(e^{\mathrm{i}\omega})]_{ij} = \frac{1}{2\pi}\int_{-\pi}^{\pi} \frac{\alpha_2^{ij}e^{4\mathrm{i}k} + \alpha_1^{ij}e^{2\mathrm{i}k} + \alpha_0^{ij}}{\beta_2 e^{4\mathrm{i}k} + \beta_1 e^{2\mathrm{i}k} + \beta_0}\mathrm{d}k \tag{5.7.16a}$$

$$= \frac{1}{2\pi}\oint_{\mathbb{S}'} \frac{\alpha_2^{ij}\mu^2 + \alpha_1^{ij}\mu + \alpha_0^{ij}}{\beta_2\mu^2 + \beta_1\mu + \beta_0}\frac{\mathrm{d}\mu}{2\mathrm{i}\mu} \tag{5.7.16b}$$

$$= \sum_{\mu_\ell\in\mathbb{D}} \mathrm{Res}\left(\frac{[R_0(e^{\mathrm{i}\omega}, \mu)]_{ij}}{\mu}, \mu_\ell\right). \tag{5.7.16c}$$

In the second to third lines we applied Cauchy's residue theorem; note that the factors of 2 cancel because with $\mu = e^{2\mathrm{i}k}$, $k \in \mathbb{T}$, we make *two* loops through the unit circle $\mathbb{S}$ (which we call $\mathbb{S}'$ above). The sum over the residues can be evaluated once we determine the roots inside the unit circle of the denominator. From the discussion above, there are several cases depending on the relation between ω and p. Below we compute the formulas for $[A(e^{\mathrm{i}\omega})]_{ij}$ together with the relations derived from result (5.7.6), namely

$$[A]_{ij} + \overline{[A]}_{ji} = \delta_{ij} \tag{5.7.17a}$$

$$[A]_{ij} - \overline{[A]}_{ji} = \mathrm{i}[H]_{ij}. \tag{5.7.17b}$$

1. Case $\cos\omega = \cos p$. There is a double pole at 0, and we find that (here $\beta = -2\sin^2\omega$)

$$\begin{aligned}[A]_{ij} &= \operatorname{Res}\left(\frac{[R_0(e^{\mathrm{i}\omega},\mu)]_{ij}}{\mu} = \frac{\alpha_2^{ij}\mu^2+\alpha_1^{ij}\mu+\alpha_0^{ij}}{\beta\mu^2}, \mu_\ell = 0\right) \\ &= -\frac{\alpha_1^{ij}}{2\sin^2\omega}.\end{aligned} \tag{5.7.18}$$

It is particular of this case that we might choose either $\omega = p$ or $\omega = -p$. Calcuations show that in either case, formula (5.7.17a) is correct. With (5.7.17b) we find

$$H = \begin{pmatrix} \cot\omega & 0 & 0 & -\mathrm{i}+\cot\omega \\ 0 & \cot\omega & 0 & \mathrm{i}-\cot\omega \\ 0 & 0 & \cot\omega & \mathrm{i}-\cot\omega \\ \mathrm{i}+\cot\omega & -\mathrm{i}-\cot\omega & -\mathrm{i}-\cot\omega & 3\cot\omega \end{pmatrix} \quad (\omega = p), \tag{5.7.19}$$

and

$$H = \begin{pmatrix} 3\cot\omega & \mathrm{i}+\cot\omega & \mathrm{i}+\cot\omega & \mathrm{i}+\cot\omega \\ -\mathrm{i}+\cot\omega & \cot\omega & 0 & 0 \\ -\mathrm{i}+\cot\omega & 0 & \cot\omega & 0 \\ -\mathrm{i}+\cot\omega & 0 & 0 & \cot\omega \end{pmatrix} \quad (\omega = -p). \tag{5.7.20}$$

In either case, the eigenvalues are

$$\begin{aligned}\sigma(H(\omega)) = \{&\cos\omega \qquad \text{(doubly degenerate)}, \\ &2\cot\omega - \sqrt{3+4\cot^2\omega},\ \ 2\cot\omega + \sqrt{3+4\cot^2\omega}\Big\}.\end{aligned} \tag{5.7.21}$$

2. Case $\cos\omega \neq \cos p$ and $|f(\omega,p)| \leq 1$. There is only a simple pole at $z = 0$. We find that (here $\beta = \cos\omega - \cos p$)

$$\begin{aligned}[A]_{ij} &= \operatorname{Res}\left(\frac{[R_0(e^{\mathrm{i}\omega},\mu)]_{ij}}{\mu} = \frac{\alpha_2^{ij}\mu^2+\alpha_1^{ij}\mu+\alpha_0^{ij}}{\beta\mu(\mu-\mu_1)(\mu-\mu_2)}, \mu_\ell = 0\right) \\ &= \frac{\alpha_0^{ij}}{\cos\omega - \cos p}.\end{aligned} \tag{5.7.22}$$

Condition (5.7.17a) does not verify. For instance, $\alpha_0^{33} + \overline{\alpha_0^{33}} = 0 \neq 1$. This case is ill-posed because there are not allowed values of $e^{\mathrm{i}\omega}$ in this region of the $(\omega,p) \in \mathbb{T}^2$ set (in the sense that $e^{\mathrm{i}\omega} \notin \sigma_{ac}(\mathcal{U})$).

3. Case $\cos\omega \neq \cos p$ and $|f(\omega,p)| > 1$. There are two poles inside $\mathbb{D}$. There are two subcases (here $\beta = \cos\omega - \cos p$).

(a) If $f(\omega, p) > 1$. Then $\mu_1 \in \mathbb{D}$, $\mu_2 \notin \mathbb{D}$. We find that

$$\begin{aligned} [A]_{ij} &= \frac{\alpha_2^{ij}\mu_1^2 + \alpha_1^{ij}\mu_1 + \alpha_0^{ij}}{\beta\mu_1(\mu_1 - \mu_2)} + \frac{\alpha_0^{ij}}{\beta} \\ &= \frac{\mu_1^2(\alpha_2^{ij} + \alpha_0^{ij}) + \mu_1\alpha_1^{ij}}{(\cos\omega - \cos p)(\mu_1^2 - 1)}. \end{aligned} \tag{5.7.23}$$

Calculations show that (5.7.17a) holds.

(b) If $f(\omega, p) < -1$. Then $\mu_1 \notin \mathbb{D}$, $\mu_2 \in \mathbb{D}$. We find that

$$\begin{aligned} [A]_{ij} &= \frac{\alpha_2^{ij}\mu_2^2 + \alpha_1^{ij}\mu_2 + \alpha_0^{ij}}{\beta\mu_2(\mu_2 - \mu_1)} + \frac{\alpha_0^{ij}}{\beta} \\ &= \frac{\mu_2^2(\alpha_2^{ij} + \alpha_0^{ij}) + \mu_2\alpha_1^{ij}}{(\cos\omega - \cos p)(\mu_2^2 - 1)}. \end{aligned} \tag{5.7.24}$$

Analogously to the previous case, calculations show that (5.7.17a) holds.

5.7.2 Power law decay

In this section we consider an interaction of infinite support. It is given by

$$V(x) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & e^{\mathrm{i}f(x)} & 0 & 0 \\ 0 & 0 & e^{\mathrm{i}f(x)} & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} \qquad \forall x \in \mathbb{Z}, \tag{5.7.25}$$

where $f : \mathbb{Z} \to \mathbb{R}^+$ is given by a power law,

$$f(x) = \frac{g}{\langle x \rangle^\alpha}, \tag{5.7.26}$$

with $0 \leq g \leq \pi$ and $\alpha > 0$. Here $x = |x_1 - x_2|$ is the relative coordinate.

The p-summability condition is explored in the following lemma.

Lemma 5.9. *With the interaction* (5.7.25)-(5.7.26)*, Assumption **(H0)** holds. Moreover, it is p-summable for $p \geq 1$ if and only if $\alpha p > 1$.*

Proof. Clearly, $f(x) \to 0$ for $|x| \to \infty$, hence $V(x) \to I_4$ in the same limit, hence $\mathcal{V}$ vanishes at infinity. It is obviously unitary, and it is radial because f is even. Hence **(H0)** holds.

To check p-summability, first consider the series

$$\sum_{x=1}^{\infty} \left(\sin \frac{g}{2x^\alpha} \right)^\beta, \tag{5.7.27}$$

with $0 \le g \le \pi$ and $\alpha, \beta \ge 0$. For $0 \le y \le \pi/2$, the bounds $\frac{2}{\pi} y \le \sin y \le y$ hold. Hence, if we let $y = \frac{g}{2x^\alpha}$ and apply the comparison test with the hyperharmonic series, then (5.7.27) converges if and only if $\alpha\beta > 1$. As shown in Proposition 5.5, $(\mathcal{V} - I) \in \mathfrak{S}_p$ if and only if the following series is finite:

$$\begin{aligned}\sum_{x\in\mathbb{Z}} \Delta^p(x) &= \sum_{x\in\mathbb{Z}} \left(\sum_{i,j} |V_{ij}(x) - \delta_{ij}|^2 \right)^{p/2} \\ &= \sum_{x\in\mathbb{Z}} \left(2|1 - e^{\mathrm{i} f(x)}|^2\right)^{p/2} \\ &= \sum_{x\in\mathbb{Z}} 8^{p/2} |\sin(f(x)/2)|^p.\end{aligned}$$

Since $f(x) = g/\langle x\rangle^\alpha$, using the summability of (5.7.27) we obtain the claim.

□

5.7.3 Repulsive interaction

We want to produce a sequence $\{V(x) : x \in \mathbb{Z}\}$ satisfying Assumption **(H0)** and that additionally has some "repulsive" behaviour at small x. Thus we require that when the particles are far ($|x| >> 1$), $V(x) \to I_4$, and when they are close, they shall interact via the Pauli matrix σ_x applied to each particle, because it changes (swaps) the direction of motion of the spin, impeding propagation.

To obtain the properties that we are looking for, the following formula is useful. Its proof, that we omit, follows from writing the series of the exponential, regrouping, and using the fact that Pauli matrices square to the identity and pairwise anticommute.

Lemma 5.10. *Let $\theta \in \mathbb{R}$ and $\vec{n} \in \mathbb{R}^3$ a unit vector, i.e. $\vec{n}^2 = 1$. Then*

$$e^{-\mathrm{i}\theta\vec{n}\cdot\vec{\sigma}} = \cos(\theta) I_2 - \mathrm{i}\sin(\theta)\vec{n}\cdot\vec{\sigma}, \tag{5.7.28}$$

where $\vec{\sigma} = (\sigma_x, \sigma_y, \sigma_z)$ are the Pauli spin matrices.

From (5.7.28), a representation of σ_x is $e^{\mathrm{i}\frac{\pi}{2}(\sigma_x - I_2)}$. This suggests how to "connect" the identity matrix and σ_x with a unitary path, via $e^{\mathrm{i}\frac{\pi}{2}\xi(\sigma_x - I_2)}$, $\xi \in [0, 1]$. Note that it evaluates to I_2 at $\xi = 0$, and to σ_x at $\xi = 1$, and it is unitary for all intermediate values of ξ. We get an explicit formula using Lemma 5.10,

$$\begin{aligned}e^{\mathrm{i}\frac{\pi}{2}\xi(\sigma_x - I_2)} &= e^{-\mathrm{i}\frac{\pi}{2}\xi}\cos(\pi\xi/2) I_2 + \mathrm{i}\sin(\pi\xi/2) e^{-\mathrm{i}\frac{\pi}{2}\xi}\sigma_x \\ &= e^{-\mathrm{i}\frac{\pi}{2}\xi}\begin{pmatrix}\cos(\pi\xi/2) & \mathrm{i}\sin(\pi\xi/2)\\ \mathrm{i}\sin(\pi\xi/2) & \cos(\pi\xi/2)\end{pmatrix}.\end{aligned} \tag{5.7.29}$$

Now define

$$V(x) = e^{\mathrm{i}\frac{\pi}{2}\xi_1(x)(\sigma_x - I_2)} \otimes e^{\mathrm{i}\frac{\pi}{2}\xi_2(x)(\sigma_x - I_2)}. \tag{5.7.30}$$

The choice $\xi_1(x) = \xi_2(x)$ corresponds to a pair of particles of the same species, and we continue with this choice from now on, and we let

$$\xi(x) = \frac{1}{\langle x \rangle^{\alpha}} \qquad \forall x \in \mathbb{Z}, \tag{5.7.31}$$

for some $\alpha > 0$.

Lemma 5.11. *With the interaction* (5.7.30)-(5.7.31)*, Assumption* ***(H0)*** *holds. Moreover, it is p-summable for $p \geq 1$ if and only if $\alpha p > 1$.*

Proof. It remains only to check the second statement. Computation gives

$$||V(x) - I_4||_F^p = 8^{p/2} |\sin y(x)|^p \, (3 - 2\sin y(x))^{p/2}\,, \tag{5.7.32}$$

where $y(x) = \frac{\pi\xi(x)}{2}$ with $\xi(x) = \langle x \rangle^{-\alpha}$. Note that $0 \leq y(x) \leq \pi/2$ for any $x \in \mathbb{Z}$. Since

$$|\sin y(x)|^p \leq |\sin y(x)|^p \, (3 - 2\sin y(x))^{p/2} \leq 5^{p/2} |\sin y(x)|^p, \tag{5.7.33}$$

comparison against (5.7.27) allows to conclude. □

5.8 Summary

Inspired by the approach in [AAM+12], we have extended the analysis of the point-interacting QW. More precisely, we have looked into several new directions:

(i) we do not restrict to Hadamard walks;

(ii) we settle the problem for interactions of arbitrary range, which depend on the spin degrees of freedom;

(iii) we propose new examples of interactions for which the methods apply.

For (i), the analysis of the free walk, though harder than in the one-dimensional case, can still be done with full generality on the parameters. Due to the link between the QWs eigenvalues, the arc length of the bands is not only controlled by r but also by the angular parts (α) and the total momentum p.

For (ii), the eigenvalue problem was formulated as the existence of solutions to a system of Fredholm integral equations of the second kind with a constraint. It was expressed in terms of the condition $1 \in \sigma(A(e^{i\omega})D(0))$, which involves $D(0) = I_4 - V(0)$ and the four-by-four matrix $A(e^{i\omega})$ which depends analytically on $e^{i\omega}$ for $e^{i\omega} \notin \sigma(\mathcal{U}_0)$.

Finally, our progress with (iii) is at a more exploratory stage. We proposed several examples and showed that they fit into the model, i.e. satisfying hypothesis **(H0)** and that are also trace-class. The natural continuation is either to attempt solving the associated system of integral equations, or to prove that it doesn't allow solutions, proving that some cases do not allow for eigenvalues. Because of its difficulty, it is to be expected that one has to resort to numerics for proceeding further. Another interesting question is to give information about the eigenvalue counting the IQW, which may be infinite in the general case.

Chapter 6

Conclusion

Our goal has been to further develop conceptually and mathematically two well-known models of computation, quantum walks and quantum cellular automata, for their potential application in quantum simulation devices, or as toy models to explore foundations of physics. Let us summarize our results and provide perspectives for future works.

6.1 Summary of results

In the first part of this thesis we quantified how good quantum walks are as simulation schemes. In **Chapter 2**, our main contribution was to provide a formal, analytic derivation of both consistency and convergence. The novelty of the approach was to import a powerful technique of numerical analysis, namely the Lax equivalence theory, in order to provide a formal proof of convergence of solutions between the QW and the associated Dirac Cauchy problem in the appropriate function spaces where it is known to be well-posed. This method avoids the trouble of previous works (e.g. [Str07]) which rely on solving the QW in order to compare its solution against that of the Dirac equation. We believe that having adapted this method is a contribution by itself: indeed, for quantum simulation schemes without known solutions, the procedure will still apply.

We also addressed the question of the discretization of the input wavefunction ϕ. Altogether we prove that for any time x_0 and a sufficiently regular initial condition ϕ, the probability of observing a discrepancy between the iterated walk Reconstruct$(W_\varepsilon^{x_0/\varepsilon}$Discretize$(\phi))$ and the solution of the Dirac equation $\psi(x_0) = T(x_0)\phi$, goes to zero, quadratically, as the discretization step ε goes to zero. Contrary to previous works, we do not limit ourselves to just consistency proof, nor to the massless case, nor to the $(1+1)$-dimensional case.

In **Chapter 3** we considered the Dirac QW, a natural candidate for being exactly discrete Lorentz covariant, given that it has the Dirac equation as continuum limit, which is of course covariant. Unfortunately, we proved the Dirac QW to be covariant only up to first-order in the lattice spacing ε. This is inconvenient if ε is considered a physically relevant quantity, i.e. if spacetime is really thought of as discrete. But if ε is thought of as an infinitesimal, then the second-order failure of Lorentz-covariance is irrelevant. Thus, this result encourages us to take the view that ε is akin to infinitesimals in non-standard analysis. Then, the Dirac QW would be understood as describing an infinitesimal time evolution, but in the same formalism as that of discrete time evolutions. As an alternative language to the Hamiltonian formalism, it has the advantage of sticking to local unitary interactions [ANW11a], and that of providing a quantum simulation algorithm.

Exact Lorentz covariance, however, is possible even for finite ε. We introduced the Clock QW, which achieves this property. However the effective dimension of its internal degree of freedom depends on the observer. Furthermore, the Clock QW does not admit a continuum limit, unless we appropriately sample the points of the lattice. Yet, its decoupled form does have a continuum limit, which is the Klein-Gordon Equation. It is interesting to see that there is a QW evolution which can be interpreted as a relativistic particle (since it satisfies the KG Equation), and yet not have a continuum limit for itself.

Actually, one may argue that the very definition of the Lorentz transform should not depend on the QW under consideration. Similarly, one may argue that the transformed wave function should be a solution of the original QW, without modifications of its parameters. However, recall that $(1+1)$ dimensional, integral Lorentz transforms are trivial unless we introduce a global rescaling. Thus the discrete Lorentz transform of this may be thought of as a biased zooming in. In order to fill in the zoomed in region, one generally has to use the QW in a weakened, reparameterized manner.

We introduced the Clock QCA, which is exactly covariant and has a three dimensional state space for its wires, and whose parameters do not depend on the scale.

In **Chapter 4** we introduced *Paired QWs*, which are both a subclass of the general QWs described above, and generalization of the most usual QWs found in the literature. Basically, *(i)* the input is allowed a simple prior encoding and *(ii)* the local unitary 'coin' is allowed to act on larger than usual neighbourhoods. Moreover, the coin is allowed to depend on space and time, as in other QW models.

We showed that Paired QWs admit as continuum limit the class of PDEs of form

$$\partial_t\psi(t,x) = B_1\partial_x\psi(t,x) + \frac{1}{2}\partial_x B_1\psi(t,x) + \mathrm{i}C\psi(t,x) \tag{6.1.1}$$

with B_1 and C hermitian and $||B_1|| \leq 1$. This class of PDEs includes the Hamiltonian form of the massive curved Dirac equation in $(1+1)$-dimensions for any bounded metric in any coordinate system, together with an electromagnetic field. Given the PDE we wish to simulate, we are able to retro-engineer the corresponding Paired QW.

Finally, in **Chapter 5** we studied the 2-particle sector of quantum cellular automata. The objective was to explore the properties and conditions of existence of discrete eigenvalues (that is, isolated eigenvalues of finite algebraic multiplicity) of the IQW. Their physical interpretation is the presence of bound states, or "molecular binding". The results extend previous works since our interactions are of arbitrary range and may act generically on the spin components. The free evolutions are generic as well. The work was organized in three steps. First, by Fourier analysis we reduced the problem to a dynamics in the the relative coordinate k only, for fixed total momentum p. We also studied in detail the spectral properties of the free walk, for generic parameters. Second, we restated the dynamic equation as a perturbation problem for interactions that are unitary, radial and vanish at infinity. Assuming a trace class condition, we provided conditions for the absence of singular continuous spectrum derived from previous works, and studied Lieb-Thirring estimates for the discrete spectrum of the perturbed walk. Third, we formulated the eigenvalue problem as a system of Fredholm integral equations of the second kind with a constraint. Finally, we revisited the contact interaction example, and proposed other examples of long range interactions that can be studied in this formalism.

6.2 Further lines of research

Developments presented in this thesis open several branches of interesting questions that may be addressed in future projects. We conclude this work by enumerating what we think are the most interesting and promising lines of future research.

1. In Chapter 2, the method could be generalized for equations of the form

$$\mathrm{i}\partial_0|\psi\rangle = D|\psi\rangle, \quad \text{with} \quad D = \sum_j D_j, \tag{6.2.1}$$

such that each $\exp(-\mathrm{i}D_j)$ is a quantum walk. Indeed, the same procedure yields the QW

$$W = \prod_j \exp(-\mathrm{i}D_j)\,. \tag{6.2.2}$$

Ultimately, it is the fact the Dirac Hamiltonian is a sum of logarithms of Quantum Walks, which enables us to model it as the product of these Quantum Walks. It would be interesting to further extend the method to non-homogeneous D_j's, for instance those considered in Chapter 5 the Dirac equation in curved spacetime.

2. The approach of Chapter 3 draws its inspiration from Quantum Information and a perspective for the future would be to discuss relativistic quantum information theory [AK84, PT04] within this framework. On the other hand, it forms part of a general trend seeking to model quantum field theoretical phenomena via discrete dynamics. For now, little is known on how to build QCA models from first principles, which admit physically relevant Hamiltonians [DP14, D'A12, Elz14, FS14b, tH13] as emergent. In this chapter we have identified one such first principle, namely the Lorentz covariance symmetry. It is interesting to study other fundamental symmetries, such as isotropy phenomena, for instance studying the propagation of circular fronts [SKT05], thereby extending our work to higher dimensions.

3. In the physical discussion of Chapter 3, we pointed out the difficulty to find other covariant models, not based on the first-order approximation nor on clocked mechanisms. This leaves the following question open: is there a systematic method which given a QW with coin operator C, decides whether it exists a Lorentz transform E_α, $f_{\alpha,\beta}$ such that $\overline{E}C_m = \overline{C}_{m'}\overline{E}$, i.e. such that the QW is covariant? The same question applies to QCA; answering it would probably confirm the intuition that covariant QWs are scarce amongst QWs.

4. In Chapter 4, we found that there is a slight overgenerality of the continuum limit that we recovered (see Eq. (6.1.1)), with respect to the $(1+1)$ curved Dirac equation, and

just matches some terms arising as $(1+1)$ projections of the $(2+1)$ curved Dirac equation. This suggests easy generalization to $(2+1)$ dimensions, through operator splitting, which is the subject of current work. For future works, the extension to $(3+1)$ dimensions remains an interesting question since gamma matrices become four dimensional. Another approach is the study the underlying symmetries of the discrete model, e.g. by making explicit some form of discrete general covariance along the same lines as [AFF14].

5. The approach adopted in Chapter 5, for the part of concrete examples, is still exploratory. For instance, one would like to find a finite range interaction (non-trivial, i.e T_G not identically zero) where the operator $(I - T_G R_0)$ can be inverted by hand. For general G this problem is standard, but not trivial; it reduces to solving a system of coupled integral equations of the second kind. In those cases numerical integration is a path to be explored.

6. Our progress with finding new examples of interactions for which the methods apply is still at a more exploratory stage. We proposed several examples and showed that they fit into the model, i.e. satisfying hypothesis **(H0)** and that are also trace-class. The natural continuation is either to attempt solving the associated system of integral equations, or to prove that it doesn't allow solutions, proving that some cases do not allow for eigenvalues. Because of its difficulty, it is to be expected that one has to resort to numerics for proceeding further. Another interesting question is to give information about the eigenvalue counting the IQW, which may be infinite in the general case.

Appendix A

Proofs for Chapter 3

A.1 Proof of the first-order-only covariance of the Dirac QW

Uniqueness of encodings. Here we prove that the only encoding compatible with first-order covariance is the flat one, as described in section 3.2.2. In general, the encoding isometries E_α, E_β can be defined in terms of normalized vectors, $\mathbf{v}_\pm$ as follows (remember that for the Dirac QW, ψ_+ and ψ_- are just scalars):

$$E_\beta \psi_+ = \psi_+ \mathbf{v}_+, \qquad E_\alpha \psi_- = \psi_- \mathbf{v}_-.$$

In order to require covariance, we need to calculate the terms appearing in the commutation relation (3.3.5). The r.h.s of the relation is (see Fig. A.1.1 and Subsection 3.2.4):

$$\overline{C}_{m'}\overline{E} = \begin{pmatrix} \psi_+\mathbf{v}_+ - im'\varepsilon(\sum \mathbf{v}_-)\psi_-\mathbf{1}_\beta \\ \psi_-\mathbf{v}_- - im'\varepsilon(\sum \mathbf{v}_+)\psi_+\mathbf{1}_\alpha \end{pmatrix} + O(\varepsilon^2)$$

where $\mathbf{1}_d = (1, \dots, 1)^\mathsf{T}$ is the d-dimensional uniform vector, and $\sum \mathbf{v} = \sum_i v_i$. On the other hand the l.h.s. is:

$$\overline{E}C_m = \begin{pmatrix} \psi_+\mathbf{v}_+ - im\varepsilon\psi_-\mathbf{v}_+ \\ \psi_-\mathbf{v}_- - im\varepsilon\psi_+\mathbf{v}_- \end{pmatrix} + O(\varepsilon^2).$$

Requiring first-order covariance, one obtains

$$m\mathbf{v}_+ = m'\left(\sum \mathbf{v}_-\right)\mathbf{1}_\beta, \qquad m\mathbf{v}_- = m'\left(\sum \mathbf{v}_+\right)\mathbf{1}_\alpha$$

which, together with the normalization of $\mathbf{v}_\pm$, gives

$$m' = \frac{m}{\sqrt{\alpha\beta}}, \quad \mathbf{v}_+ = \frac{e^{i\lambda_+}}{\sqrt{\beta}}\mathbf{1}_\beta, \quad \mathbf{v}_- = \frac{e^{i\lambda_-}}{\sqrt{\alpha}}\mathbf{1}_\alpha.$$

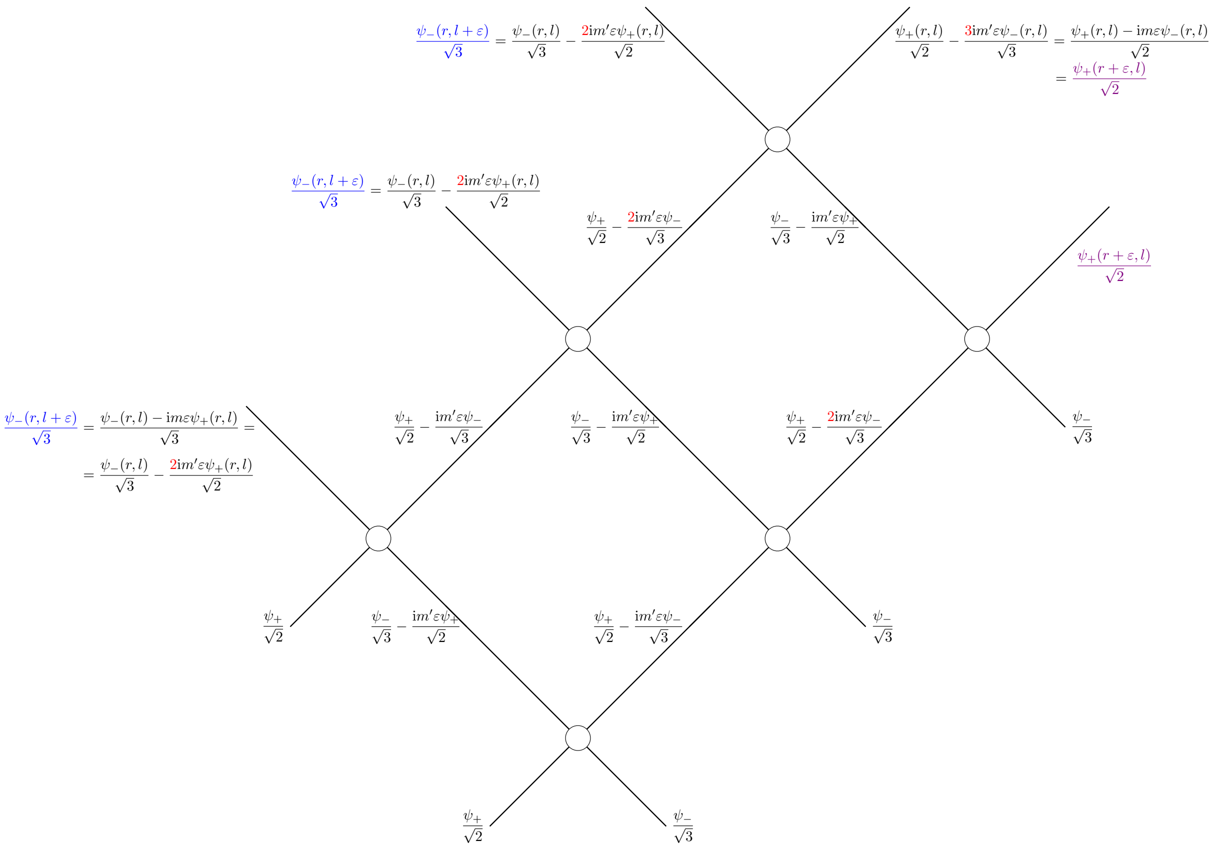


Figure A.1.1: *First order covariance of the Dirac QW*. In the first order, the outcoming wires of a patch match the incoming wires of the next patch. Unless otherwise indicated, all the fields values appearing in this Figure are evaluated at (r, l).

thereby proving that the only possible encoding compatible with first-order covariance is the flat one (up to irrelevant phases).

A.2 Failure at second order

The Dirac QW can similarly be expanded to the second order. This time, however, the patches that make up ψ' do not match up. A simple counter-example supporting this fact arises with $\alpha = 2$ and $\beta = 1$ already, as illustrated in Fig. A.2.1. Notice that we ought to have $\overline{C}(0,1)\breve{\psi}_-(0,0) = \overline{C}(1,1)\breve{\psi}_-(0,0)$, if we want those outcoming wires to match up with the corresponding incoming wires of the next patch $\breve{\psi}_-(0,1)_0 = \breve{\psi}_-(0,1)_1 = \psi_-(0,1)/\sqrt{2}$. But it turns out that those outcoming wires verify

$$\overline{C}(0,1)\breve{\psi}_-(0,0) \neq \overline{C}(1,1)\breve{\psi}_-(0,0) \tag{A.2.1}$$

due a term in ε^2.

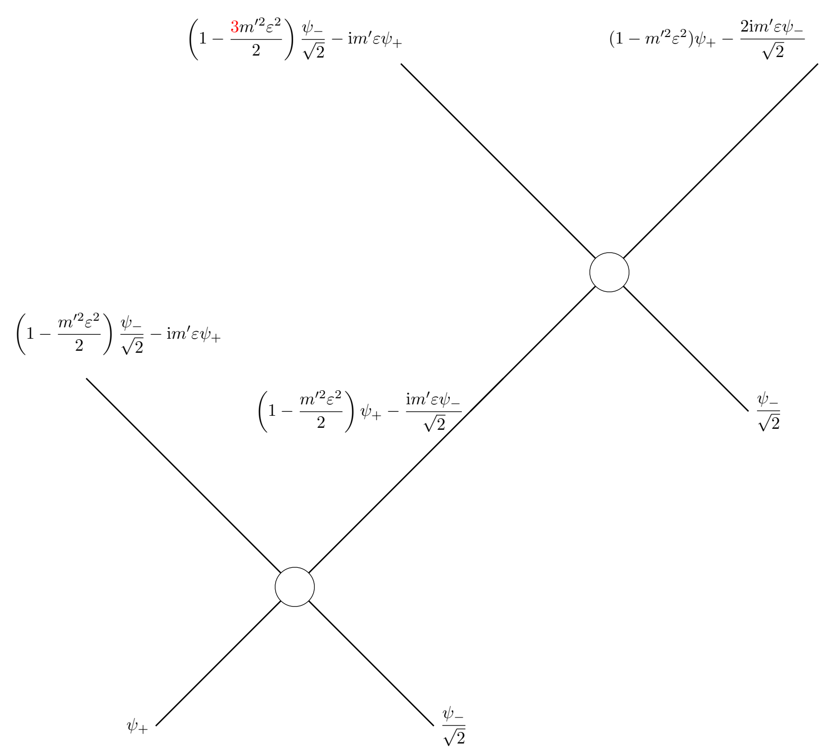


Figure A.2.1: *Failure of covariance at the second order for the Dirac QW.* The outcoming wires of a patch do not match the incoming wires of the next patch.

Appendix B

Proofs for Chapter 4

B.1 Calculation of the first order expansion of the discrete model

In this section we prove Eq. (4.2.11), which we reproduce here:

$$\begin{bmatrix} 2\varepsilon\partial_t u \\ 2\varepsilon\partial_t d \\ u' \\ d' \end{bmatrix} = (I \oplus U) \begin{bmatrix} 0 \\ 0 \\ u' \\ d' \end{bmatrix} + (I \oplus U)B \begin{bmatrix} 2u' \\ 2d' \\ 0 \\ 0 \end{bmatrix}$$
$$+ \varepsilon \left\{ (2N - \mathrm{i}\tilde{E})(I \oplus U) + (I \oplus U)(\mathrm{i}\tilde{E} + 2M) + T \right\} \begin{bmatrix} u \\ d \\ 0 \\ 0 \end{bmatrix}. \tag{B.1.1}$$

Recall that we want to expand

$$\phi_{out}(t,x) = G\, \phi_{in}(t,x), \tag{B.1.2}$$

where

$$G = E^{\dagger}(t+2,x)W'(t,x)(P' \oplus P)(E(t,x-2) \oplus E(t,x+2)). \tag{B.1.3}$$

The first order expansion of the encoding and of the walk is, by definition,

$$E(t,x) = E^{(0)}(t,x) + \varepsilon \mathrm{i} E^{(0)}(t,x)\tilde{E}(t,x) + O(\varepsilon^2) \tag{B.1.4}$$
$$W'(t,x) = W^{(0)}(t,x) + \varepsilon \mathrm{i} W^{(0)}(t,x)\tilde{W}(t,x) + O(\varepsilon^2), \tag{B.1.5}$$

hence, to first order in ε, the operators in (B.1.3) expand to

$$E^\dagger(t+2,x) \simeq E^{(0)\dagger} + \varepsilon\left(2\partial_t E^{(0)\dagger} - \mathrm{i}\tilde{E}E^{(0)\dagger}\right) \tag{B.1.6}$$

$$W'(t,x) \simeq W^{(0)} + \varepsilon \mathrm{i} W^{(0)}\tilde{W} \tag{B.1.7}$$

$$E(t,x-2) \oplus E(t,x+2) \simeq \left(E^{(0)} - 2\varepsilon\partial_x E^{(0)} + \mathrm{i}\varepsilon E^{(0)}\tilde{E}\right) \oplus \left(E^{(0)} + 2\varepsilon\partial_x E^{(0)} + \mathrm{i}\varepsilon E^{(0)}\tilde{E}\right). \tag{B.1.8}$$

In the right hand side all operators are evaluated at (t,x). Recall that the first order expansions of the output and the input are

$$\phi_{out}(t,x) \simeq \begin{bmatrix} u \\ d \\ 0 \\ 0 \end{bmatrix} + \begin{bmatrix} 2\varepsilon\partial_t u \\ 2\varepsilon\partial_t d \\ u' \\ d' \end{bmatrix}, \qquad \phi_{in}(t,x) \simeq \begin{bmatrix} u \\ d \\ 0 \\ 0 \end{bmatrix} \oplus \begin{bmatrix} u \\ d \\ 0 \\ 0 \end{bmatrix} + \begin{bmatrix} -2u' \\ -2d' \\ u' \\ d' \end{bmatrix} \oplus \begin{bmatrix} 2u' \\ 2d' \\ u' \\ d' \end{bmatrix}. \tag{B.1.9}$$

We shall use the identities

$$(P' \oplus P)(E \oplus E)(v \oplus v) = XEv \tag{B.1.10}$$

$$(P' \oplus P)(E \oplus E)(-v \oplus v) = XZEv \tag{B.1.11}$$

valid for any $v \in \mathbb{C}^4$, because P' (resp. P) are the projections onto the primed (resp. non-primed) coordinates; in matrix form,

$$P' = \begin{pmatrix} 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \qquad P = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{pmatrix}. \tag{B.1.12}$$

Next we plug the previous expansions into (B.1.2). Collecting all the terms of first order in ε,

$$\begin{aligned} \begin{bmatrix} 2\varepsilon\partial_t u \\ 2\varepsilon\partial_t d \\ u' \\ d' \end{bmatrix} &= E^{(0)\dagger}W^{(0)}XE^{(0)} \begin{bmatrix} 0 \\ 0 \\ u' \\ d' \end{bmatrix} + E^{(0)\dagger}W^{(0)}XZE^{(0)} \begin{bmatrix} 2u' \\ 2d' \\ 0 \\ 0 \end{bmatrix} \\ &+ \Big\{\varepsilon(2\partial_t E^{(0)\dagger} - \mathrm{i}\tilde{E}E^{(0)\dagger})W^{(0)}XE^{(0)} + \mathrm{i}\varepsilon E^{(0)\dagger}W^{(0)}\tilde{W}XE^{(0)} + \mathrm{i}\varepsilon E^{(0)\dagger}W^{(0)}XE^{(0)}\tilde{E} \\ &+ 2\varepsilon E^{(0)\dagger}W^{(0)}XZ\partial_x E^{(0)}\Big\} \begin{bmatrix} u \\ d \\ 0 \\ 0 \end{bmatrix}. \end{aligned}$$

Next we use the zeroth order condition (cf. (4.2.10)), namely $E^{(0)\dagger}W^{(0)}XE^{(0)} = I \oplus U$, so that

$$\begin{aligned}\begin{bmatrix}2\varepsilon\partial_t u\\ 2\varepsilon\partial_t d\\ u'\\ d'\end{bmatrix} = (I\oplus U)\begin{bmatrix}0\\0\\u'\\d'\end{bmatrix} + (I\oplus U)\underbrace{E^{(0)\dagger}ZE^{(0)}}_{\mathrm{B}}\begin{bmatrix}2u'\\2d'\\0\\0\end{bmatrix}\\ \varepsilon\left\{\left[2\underbrace{(\partial_t E^{(0)\dagger})E^{(0)}}_{\mathrm{N}} - \mathrm{i}\tilde{E}\right](I\oplus U) + \underbrace{\mathrm{i}E^{(0)\dagger}W^{(0)}\tilde{W}XE^{(0)}}_{\mathrm{T}}\right.\\ \left. + \mathrm{i}(I\oplus U)\tilde{E} + 2(I\oplus U)\underbrace{E^{(0)\dagger}Z\partial_x E^{(0)}}_{\mathrm{M}}\right\}\begin{bmatrix}u\\d\\0\\0\end{bmatrix},\end{aligned}$$

and we get the desired result.

B.2 General form of B

Since B must be hermitian, cf. (4.2.12a), then B_1 and B_4 are hermitian. Since it is also unitary, then it must square to the identity. This implies that the conditions

$$B_1^2 + B_2^\dagger B_2 = \mathrm{Id}_2 \tag{B.2.1a}$$

$$B_4^2 + B_2 B_2^\dagger = \mathrm{Id}_2 \tag{B.2.1b}$$

and

$$B_2 B_1 + B_4 B_2 = 0 \tag{B.2.2a}$$

$$B_1 B_2^\dagger + B_2^\dagger B_4 = 0 \tag{B.2.2b}$$

must hold. Note also that B must have a complete set of orthonormal eigenvectors, eigenvalues ± 1, and it shall be traceless, because it is is similar to Z.

First, we parametrize the block B_2. Consider the spectral decomposition of $B_1 = VDV^\dagger$, $D = \mathrm{diag}\{d_1, d_2\}$. From the first of conditions (B.2.1a), we have that $d_1, d_2 \in [-1, 1]$, because the square root of the components of $\mathrm{Id} - D^2$ are precisely the singular values of B_2, which should be non-negative. Next, we shall find B_2 such that constraint (4.2.25a) is satisfied. The same equation also determines U.

We look for $B_2 \in \mathbb{C}^{2\times 2}$ such that conditions (4.2.25a) and (B.2.1a) are satisfied, namely that

1. $\mathrm{Id} + 2B_2$ is unitary,
2. $B_2^\dagger B_2 = \mathrm{Id} - B_1^2$.

To prove our lemma we will use a shortcut provided by the following characterization of matrices with positive definite [Bha09] real part. Recall that if $A \in \mathbb{C}^{n\times n}$, its real and imaginary parts are $\Re A := \frac{1}{2}(A + A^\dagger)$ and $\Im A = \frac{1}{2\mathrm{i}}(A - A^\dagger)$, respectively.

Theorem B.1 (see [Lon81]). *Let $A \in \mathbb{C}^{n\times n}$. Then, $\Re A$ is positive definite if and only if*

$$A = T \begin{pmatrix} 1+\mathrm{i}\alpha_1 & & \\ & \ddots & \\ & & 1+\mathrm{i}\alpha_n \end{pmatrix} T^\dagger \tag{B.2.3}$$

for some non-singular T and $\alpha_1, \dots, \alpha_n \in \mathbb{R}$.

Note that, from condition 1 above,

$$(\mathrm{Id} + 2B_2^\dagger)(\mathrm{Id} + 2B_2) = \mathrm{Id} \Rightarrow B_2 + B_2^\dagger + 2(B_2^\dagger B_2) = 0, \tag{B.2.4}$$

hence condition 1 is equivalent to $\Re B_2 = -B_2^\dagger B_2$. Recall that $A^\dagger A$ is positive definite for any $A \in \mathbb{C}^{n\times n}$, hence Theorem B.1 can be applied to $-B_2$.

We recall the following parametrization of the $U(2)$ group, namely that

$$U(2) = \left\{ e^{\mathrm{i}\theta} \begin{pmatrix} \alpha & \beta \\ -\overline{\beta} & \overline{\alpha} \end{pmatrix} : \theta \in [0, 2\pi),\ \alpha, \beta \in \mathbb{C},\ |\alpha|^2 + |\beta|^2 = 1 \right\}. \tag{B.2.5}$$

Lemma B.1. *Let $B_1 \in \mathbb{C}^{2\times 2}$ be hermitian, with spectral decomposition $B_1 = V_1 D_1 V_1^\dagger$, and eigenvalues $d_1, d_2 \in [-1, 1] \in \mathbb{R}$. Assume that $B_2 \in \mathbb{C}^{2\times 2}$ satisfies the conditions*

1. $\Re B_2 = -B_2^\dagger B_2$,
2. $B_2^\dagger B_2 = \mathrm{Id} - B_1^2$.

Then,

$$B_2 = -K \begin{pmatrix} \lambda_1 e^{\mathrm{i}\eta_1^\pm} & 0 \\ 0 & \lambda_2 e^{\mathrm{i}\eta_2^\pm} \end{pmatrix} K^\dagger, \tag{B.2.6}$$

where $\lambda_i = \sqrt{1-d_i^2}$, $\sin\eta_i^\pm = \pm|d_i|$, $-\pi/2 \le \eta_i^\pm \le \pi/2$, $i \in \{1,2\}$. If $d_1^2 \neq d_2^2$ (non-degenerate case) then $K = V_1$, if $d_1^2 = d_2^2$ (degenerate case) then $K \in U(2)$ is arbitrary.

Proof. From Theorem B.1, and condition 1, B_2 can be written as $B_2 = -T_2 D_2 T_2^\dagger$ for some non-singular T_2 and $D_2 = \mathrm{diag}\{1+\mathrm{i}\alpha_1, 1+\mathrm{i}\alpha_2\}$, $\alpha_1, \alpha_2 \in \mathbb{R}$. Substitution into condition 1 gives

$$T_2^\dagger T_2 = \begin{pmatrix} (1+\alpha_1^2)^{-1} & 0 \\ 0 & (1+\alpha_2^2)^{-1} \end{pmatrix}. \tag{B.2.7}$$

Now, let the SVD of $T_2 = W\Sigma V^\dagger$. Then $T_2^\dagger T_2 = V\Sigma^2 V^\dagger$ and using (B.2.7) it is easy to see, using the canonical decomposition of unitary matrices (cf. (B.2.5)), that we must have one of the following cases:

1. If $\alpha_1^2 \neq \alpha_2^2$, then for some $\theta_1, \theta_2 \in [0, 2\pi)$, either

(a) $\Sigma = \begin{pmatrix} \frac{1}{\sqrt{1+\alpha_2^2}} & 0 \\ 0 & \frac{1}{\sqrt{1+\alpha_1^2}} \end{pmatrix}$ and $V = \begin{pmatrix} 0 & e^{\mathrm{i}\theta_1} \\ e^{\mathrm{i}\theta_2} & 0 \end{pmatrix}$. Hence,

$$B_2 = -W \begin{pmatrix} \frac{1+\mathrm{i}\alpha_2}{1+\alpha_2^2} & 0 \\ 0 & \frac{1+\mathrm{i}\alpha_1}{1+\alpha_1^2} \end{pmatrix} W^\dagger.$$

(b) $\Sigma = \begin{pmatrix} \frac{1}{\sqrt{1+\alpha_1^2}} & 0 \\ 0 & \frac{1}{\sqrt{1+\alpha_2^2}} \end{pmatrix}$ and $V = \begin{pmatrix} e^{\mathrm{i}\theta_1} & 0 \\ 0 & e^{\mathrm{i}\theta_2} \end{pmatrix}$. Hence,

$$B_2 = -W \begin{pmatrix} \frac{1+\mathrm{i}\alpha_1}{1+\alpha_1^2} & 0 \\ 0 & \frac{1+\mathrm{i}\alpha_2}{1+\alpha_2^2} \end{pmatrix} W^\dagger.$$

Note that in either case, we can write $B_2 = -W \operatorname{diag}\left\{ \frac{1+\mathrm{i}\alpha_{\sigma(1)}}{1+\alpha_{\sigma(1)}^2}, \frac{1+\mathrm{i}\alpha_{\sigma(2)}}{1+\alpha_{\sigma(2)}^2} \right\} W^\dagger$, where $\sigma : \{1,2\} \to \{1,2\}$ is a permutation. It is easy to check that condition 1 is indeed satisfied. Next, substitution into condition 2 gives

$$\begin{pmatrix} 1-d_1^2 & 0 \\ 0 & 1-d_2^2 \end{pmatrix} = K \begin{pmatrix} \frac{1}{1+\alpha_{\sigma(1)}^2} & 0 \\ 0 & \frac{1}{1+\alpha_{\sigma(2)}^2} \end{pmatrix} K^\dagger, \tag{B.2.8}$$

with $K := V_1^\dagger W \in U(2)$. Again, we use the canonical form, cf. (B.2.5), to find that K is diagonal or antidiagonal, with two independent phases. Introducing back W into B_2, in either case we have $\alpha_i^2 = \frac{d_i^2}{1-d_i^2}$, $i = 1, 2$, hence $\alpha_i = \pm\frac{|d_i|}{\sqrt{1-d_i^2}}$, so

$$\frac{1+\mathrm{i}\alpha_i}{1+\alpha_i^2} = \sqrt{1-d_i^2}\left(\sqrt{1-d_i^2} \pm \mathrm{i}|d_i|\right) = \sqrt{1-d_i^2}\, e^{\mathrm{i}\eta_i^\pm}, \tag{B.2.9}$$

provided that $\cos\eta_i^\pm = \sqrt{1-d_i^2}$, and $\sin\eta_i^\pm = \pm|d_i|$. This proves part 1.

2. If $\alpha_1^2 = \alpha_2^2$, then $\Sigma = \frac{1}{\sqrt{1+\alpha_1^2}} \mathrm{Id}_2$, and $V \in U(2)$ is arbitrary. Thus, we can write $B_2 = -\frac{1}{1+\alpha_1^2} K \begin{pmatrix} 1+\mathrm{i}\alpha_1 & 0 \\ 0 & 1 \pm \mathrm{i}\alpha_1 \end{pmatrix} K^\dagger$ for some $K \in U(2)$. Substitution into condition 2, gives $\alpha_1^2 = d_1^2/(1-d_1^2)$, and proceeding as in (B.2.9), we obtain the claim.

□

Next we characterize B_4. We assume that the relevant constraints fron (B.2.1a)-(B.2.2b) are satisfied, namely $B_1^2 + B_2^\dagger B_2 = \mathrm{Id}_2$ and that $B_4^2 + B_2 B_2^\dagger = \mathrm{Id}_2$.

Lemma B.2. *In the hypothesis of above,*

1. *If $d_1^2 \neq d_2^2$ (non-degenerate case), then $B_4 = -B_1$.*

2. *If $d_1^2 = d_2^2$ (degenerate case),*

$$B_4 = -sK' \begin{pmatrix} d_1 & 0 \\ 0 & d_2 \end{pmatrix} K'^{\dagger}, \tag{B.2.10}$$

   where $K' \in U(2)$ is arbitrary and $s = 1$ if $d_1 = d_2$, $s = \pm 1$ if $d_1 = -d_2$.

Proof. From (4.2.25a), B_2 is normal, then from (B.2.1a) and (B.2.1b) we have that $B_1^2 = B_4^2$. Since B_4 is hermitian consider its spectral decomposition, $B_4 = WD_4W^{\dagger}$, $W \in U(2)$. Then, $D_4^2 = KD_1^2K^{\dagger}$, where $K := W^{\dagger}V_1$. Using the canonical form (B.2.5), we find that

1. If $d_1^2 \neq d_2^2$, then K is either diagonal or anti-diagonal, with arbitrary phases. In either case we obtain $B_4 = V_1 \mathrm{diag}\{\pm d_1, \pm d_2\} V_1^{\dagger}$, but since we must have $\mathrm{Tr} B_4 = -\mathrm{Tr} B_1$, we shall take $-d_1$, $-d_2$. Hence, $B_4 = -B_1$.

2. If $d_1^2 = d_2^2$, then $K \in U(2)$ is arbitrary, and we have $B_4 = V_1 K^{\dagger} \mathrm{diag}\{\pm d_1, \pm d_1\} K V_1^{\dagger}$. If $d_1 = d_2$, then $\mathrm{Tr} B_4 = -2d_1$, so $B_4 = -d_1 \, \mathrm{Id}_2$. If $d_1 = -d_2$, then $\mathrm{Tr} B_4 = 0$, and we can take $d_1, -d_1$ or $-d_1, d_1$.

□

Appendix C

Complement to Chapter 5

C.1 Review of distribution theory in $\mathbb{T}^n$

In this section we recall some notation from distribution theory and standard results from Fourier analysis. For preparing this section, useful references treating periodic distributions were [Sch61a, Zem82], though we mainly follow the lecture notes by M. Salo [Sal13].

The space of *rapidly decreasing sequences* is denoted $\mathcal{S}(\mathbb{Z}^n)$. Recall that a sequence $\psi = \{\psi(x)\}_{x\in\mathbb{Z}^n} \subset \mathbb{C}$ is said to be rapidly decreasing if for any $N > 0$ there is $c_N > 0$ such that

$$|\psi(x)| \leq c_N \langle x \rangle^{-N} \tag{C.1.1}$$

for all $x \in \mathbb{Z}^n$. We equip $\mathcal{S}(\mathbb{Z}^n)$ with the topology induced by the norms

$$\psi \mapsto \sup_{x\in\mathbb{Z}^n} \langle x \rangle^N |\psi(x)|. \tag{C.1.2}$$

Note that $\mathcal{S}(\mathbb{Z}^n)$ is a discrete analogue of $\mathcal{S}(\mathbb{R}^n)$, the Schwartz space of rapidly decreasing functions, i.e. $\mathcal{S}(\mathbb{R}^n) = \{f \in \mathbb{C}^\infty(\mathbb{R}^n) : \forall \alpha, \beta \in \mathbb{N}_0^n \ \ ||f||_{\alpha,\beta} < \infty\}$, where $||f||_{\alpha,\beta} = ||x^\alpha D^\beta f||_{L^\infty(\mathbb{R}^n)}$.

The space of *periodic test functions*, noted $\mathcal{P}(\mathbb{R}^n)$, is the set of all infinitely differentiable functions $\mathbb{R}^n \to \mathbb{C}$ that are 2π-periodic in each variable. A sequence $\{\hat{\varphi}_j\}_{j\in\mathbb{N}} \subset \mathcal{P}(\mathbb{R}^n)$ converges to $\hat{\varphi}$ if for all $\alpha \in \mathbb{N}_0^n$, $\partial^\alpha \hat{\varphi}_j \to \partial^\alpha \hat{\varphi}$ uniformly in $\mathbb{R}^n$.

We denote by $\mathcal{F}$ the Fourier series, given by the following map:

$$\mathcal{F} : \mathcal{S}(\mathbb{Z}^n) \to \mathcal{P}(\mathbb{R}^n), \qquad \psi \mapsto \hat{\psi}(k) = \sum_{x\in\mathbb{Z}^n} \psi(x) e^{-\mathrm{i}k\cdot x}. \tag{C.1.3}$$

Conversely, the inverse Fourier map $\mathcal{F}^{-1}$ is the Fourier series of test functions, taking a test function to its sequence of Fourier coefficients,

$$\mathcal{F}^{-1} : \mathcal{P}(\mathbb{R}^n) \to \mathcal{S}(\mathbb{Z}^n), \ \ \hat{\psi} \mapsto \psi = \{\psi(x)\}_{x\in\mathbb{Z}^n}, \ \psi(x) = \frac{1}{(2\pi)^n} \int_{\mathbb{T}^n} \hat{\psi}(k) e^{\mathrm{i}k\cdot x} \mathrm{d}k. \tag{C.1.4}$$

It is important to recall that the map $\mathcal{F}$ is an isomorphism between $\mathcal{S}(\mathbb{Z}^n)$ and $\mathcal{P}(\mathbb{R}^n)$, and any periodic test function $\hat{\psi} \in \mathcal{P}(\mathbb{R}^n)$ can be written as the Fourier series of some sequence, as in the right-hand side of (C.1.3), with convergence in $\mathcal{P}(\mathbb{R}^n)$.

Remark C.1. We recall that any function in $L^2(\mathbb{T}^n)$ can be approximated with arbitrary accuracy (in L^2-norm) with a sequence of functions in $\mathcal{P}(\mathbb{R}^n)$. Indeed, any continuous function on $\mathbb{T}^n$ can be approximated uniformly by trigonometric polynomials, and since uniform convergence on $\mathbb{T}^n$ implies L^2 convergence and continuous functions are dense in $L^2(\mathbb{T}^n)$, it follows that $\mathcal{P}(\mathbb{R}^n)$ is dense in $L^2(\mathbb{T}^n)$. The theory of Fourier series of L^2 functions can be defined as in Eqs. (C.1.3) and (C.1.4), this time acting between the spaces $\mathcal{F} : \ell^2(\mathbb{Z}^n) \to L^2(\mathbb{T}^n)$, where convergence of the Fourier series is understood in the sense of L^2.

The main properties of the Fourier series of periodic test functions are summarized below. We use $(\psi)^\wedge(k)$ to denote the Fourier series of the sequence $\psi = \{\psi(x)\}_{x\in\mathbb{Z}^n}$ evaluated at k, that is, $(\psi)^\wedge(k) = \hat{\psi}(k)$.

Theorem C.1. *(properties of the Fourier series on $\mathcal{P}$). Let $\psi \in \mathcal{S}(\mathbb{Z}^n)$, then the following properties hold:*

1. *translation:* $(\tau_{x_0}\psi)^\wedge(k) = e^{-\mathrm{i}k\cdot x_0}\hat{\psi}(k)$, $x_0 \in \mathbb{Z}^n$.
2. *modulation:* $(e^{\mathrm{i}k_0\cdot x}\psi(x))^\wedge(k) = (\tau_{k_0}\hat{\psi})(k)$, $k_0 \in \mathbb{T}^n$.
3. *derivative:* $((-1)^{|\alpha|}(x)^\alpha\psi(x))^\wedge(k) = (D^\alpha\hat{\psi})(k)$, $\alpha \in \mathbb{N}_0^n$.
4. *product:* $(\psi\varphi)^\wedge(k) = (\hat{\psi} * \hat{\varphi})(k)$, *with convolution in $\mathcal{P}$ being* $(\hat{\psi} * \hat{\varphi})(k) = (2\pi)^{-n}\int_{\mathbb{T}^n}\hat{\psi}(k-k')\hat{\varphi}(k')\mathrm{d}k'$.
5. *convolution:* $((\psi * \varphi)(x))^\wedge(k) = (\hat{\psi}\hat{\varphi})(k)$, *with discrete convolution being* $(\psi * \varphi)(x) = \sum_{x'\in\mathbb{Z}^n}\psi(x-x')\varphi(x')$.

The space of sequences of polynomial growth, or *slow growth*, is denoted with $\mathcal{S}'(\mathbb{Z}^n)$. Recall that a complex sequence $\psi = \{\psi(x)\}_{x\in\mathbb{Z}^n}$ is said to be of slow growth if there exists $N > 0$ and $c > 0$ such that

$$|\psi(x)| \leq c\langle x\rangle^N \tag{C.1.5}$$

for all $x \in \mathbb{Z}^n$.

The space of *periodic distributions*, noted $\mathcal{P}'$, is the set of all continuous linear functionals on $\mathcal{P}$, that is,

$$\mathcal{P}' = \left\{\hat{T} : \mathcal{P} \to \mathbb{C}; \hat{T} \text{ is linear and } \hat{T}(\hat{\varphi}_j) \to 0 \text{ if } \hat{\varphi}_j \to 0 \text{ in } \mathcal{P}\right\}. \tag{C.1.6}$$

For example, each periodic test function that is Lebesgue integrable, $\hat{\varphi} \in L^1(\mathbb{T}^n)$, induces a unique (as an element of $\mathcal{P}'$) periodic distribution, if we set

$$\hat{T}_{\hat{\varphi}} : \mathcal{P} \to \mathbb{C}, \qquad \hat{\varphi} \mapsto \int_{\mathbb{T}^n}\hat{\varphi}\,\hat{\psi}\,\mathrm{d}k. \tag{C.1.7}$$

An advantage of this identification is that operations on $\mathcal{P}$ can be defined on $\mathcal{P}'$ by duality. Another example is given by any finite complex Borel measure μ on $\mathbb{R}^n$ that is periodic, in the sense that $\mu(E + 2\pi e_j) = \mu(E)$, for any Borel set $E \subset \mathbb{R}^n$ and e_j is an element of the canonical basis of $\mathbb{R}^n$. In this case we integrate against the measure,

$$\hat{T}_\mu(\hat{\varphi}) = \int_{\mathbb{T}^n} \hat{\varphi}\,\mathrm{d}\mu. \tag{C.1.8}$$

An important case is given by the Dirac delta measure, that satisfies $\hat{T}_\delta(\hat{\varphi}) = \hat{\varphi}(0)$, and is defined for any Borel set $E \subset \mathbb{R}^n$ as

$$\delta(E) = \begin{cases} 1, & \text{if } E \cap 2\pi\mathbb{Z}^n \neq \emptyset \\ 0, & \text{otherwise} \end{cases} \tag{C.1.9}$$

The Dirac delta on $\mathcal{P}'(\mathbb{R})$ is also written as $\sum_{x\in\mathbb{Z}} \delta(k - 2\pi x)$, $k \in \mathbb{T}$.

Next we consider *Fourier series of periodic distributions*. If $\hat{T} \in \mathcal{P}'(\mathbb{R}^n)$ is a periodic distribution, its Fourier coefficients are defined as

$$T(x) := (2\pi)^{-n}\hat{T}(e^{\mathrm{i}kx}), \qquad x \in \mathbb{Z}^n. \tag{C.1.10}$$

The central result is that any periodic distribution has a Fourier series that converges in the sense of distributions. This provides a weak notion for convergence of trigonometric series that we shall apply when dealing with the interaction operator $\mathcal{V}$. More precisely, it can be proved that any $\hat{T} \in \mathcal{P}'$ can be written as the Fourier series

$$\hat{T} = \sum_{x\in\mathbb{Z}^n} T(x)e^{-\mathrm{i}k\cdot x}, \tag{C.1.11}$$

whith convergence in the sense of distributions, i.e.

$$\left(\lim_{N\to\infty} \sum_{|k|\leq N} T(x)e^{-\mathrm{i}k\cdot x}\right)(\hat{\varphi}) = \hat{T}(\hat{\varphi}) \tag{C.1.12}$$

for arbitrary $\hat{\varphi} \in \mathcal{P}$. Conversely, any sequence of slow growth induces a periodic distribution via (C.1.11). In this sense the Fourier map (C.1.10) defines a bijection between the spaces $\mathcal{P}'(\mathbb{R}^n)$ and $\mathcal{S}'(\mathbb{Z}^n)$.

Example C.1.1. Consider the Dirac delta measure $\delta \in \mathcal{P}'(\mathbb{R}^n)$ introduced above. From definition (C.1.10), its Fourier coefficients are $(2\pi)^{-n}$ for all $x \in \mathbb{Z}^n$, and using (C.1.11) we obtain the *Poisson summation formula*,

$$\sum_{x\in\mathbb{Z}^n} e^{-\mathrm{i}k\cdot x} = (2\pi)^n \sum_{x\in\mathbb{Z}^n} \delta(k - 2\pi x), \qquad k \in \mathbb{T}^n. \tag{C.1.13}$$

Below we summarize the properties of the Fourier series of periodic distributions, which are in some sense dual of those presented in Theorem (C.1).

Theorem C.2. *(properties of the Fourier series on $\mathcal{P}'$). Let $\hat{\varphi} \in \mathcal{P}(\mathbb{R}^n)$ and $\hat{T} \in \mathcal{P}'(\mathbb{R}^n)$, then the following properties hold:*

1. *translation:* $(\tau_{x_0}T(x))^\wedge(k) = e^{-\mathrm{i}k\cdot x_0}\hat{T}(k)$, $x_0 \in \mathbb{Z}^n$.

2. *modulation:* $(e^{\mathrm{i}k_0\cdot x}T(x))^\wedge(k) = (\tau_{k_0}\hat{T})(k)$, $k_0 \in \mathbb{T}^n$.

3. *weak derivative:* $((-1)^{|\alpha|}x^\alpha T(x))^\wedge(k) = (D^\alpha\hat{T})(k)$, $\alpha \in \mathbb{N}_0^n$.

4. *convolution:* $((T * \varphi)(x))^\wedge(k) = (\hat{T}\hat{\varphi})(k)$.

5. *product:* $(T\varphi)^\wedge(k) = (\hat{T} * \hat{\varphi})(k)$.

Below is a summary of operations on $\mathcal{P}'$ that can be defined by duality with $\mathcal{P}$.

Theorem C.3. *(operations on $\mathcal{P}'$). Let $\hat{\psi}, \hat{\varphi} \in \mathcal{P}(\mathbb{R}^n)$ and $\hat{T} \in \mathcal{P}'(\mathbb{R}^n)$. Then the following operations are well defined:*

1. *reflection:* $\tilde{\hat{T}}(\hat{\varphi}) = \hat{T}(\tilde{\hat{\varphi}})$, *where* $\tilde{\hat{\varphi}}(k) = \hat{\varphi}(-k)$.

2. *conjugation:* $\overline{\hat{T}}(\hat{\varphi}) = \overline{\hat{T}(\overline{\hat{\varphi}})}$.

3. *translation:* $(\tau_{k_0}\hat{T})(\hat{\varphi}) = \hat{T}(\tau_{-k_0}\hat{\varphi})$, $k_0 \in \mathbb{T}^n$.

4. *weak derivative:* $(\partial^\alpha\hat{T})(\hat{\varphi}) = (-1)^{|\alpha|}\hat{T}(\partial^\alpha\hat{\varphi})$, $\alpha \in \mathbb{N}_0^n$.

5. *product:* $(\hat{\psi}\hat{T})(\hat{\varphi}) = \hat{T}(\hat{\psi}\hat{\varphi})$.

6. *convolution:* $(\hat{T} * \hat{\psi})(\hat{\varphi}) = \hat{T}(\tilde{\hat{\psi}} * \hat{\varphi})$.

Next we present more properties of the Fourier series of periodic distributions and a structure theorem, which states that periodic distributions always arise as a distributional derivative of a continuous periodic function.

Theorem C.4. *Let $\hat{T} \in \mathcal{P}'$ be arbitrary. Then:*

1. *It has finite order, i.e. there exist $N > 0$ and $c > 0$ such that*

$$|\hat{T}(\hat{\varphi})| \leq c \sum_{|\alpha|\leq N} ||\partial^\alpha\hat{\varphi}||_{L^\infty} \tag{C.1.14}$$

2. *It is uniquely determined by its Fourier coefficients, i.e. if $T(x) = 0$ for all $x \in \mathbb{Z}^n$, then $\hat{T} = 0$.*

Theorem C.5. *(structure theorem for periodic distributions). Any periodic distribution $\hat{T} \in \mathcal{P}'$ may be expressed as*

$$\hat{T} = (1 - \nabla^2)^N\hat{\xi}, \tag{C.1.15}$$

for some continuous 2π-periodic $\hat{\xi}$ in $\mathbb{R}^n$ and some integer $N \geq 0$, and $\nabla^2 = \sum_{j=1}^n \frac{\partial^2}{\partial x_j^2}$ is the Laplacian operator.

C.2 Review of spectral theory in Hilbert space

We denote by $\mathcal{L}(\mathcal{H})$ the algebra of bounded linear operators in a complex, separable Hilbert space $\mathcal{H}$. If $A \in \mathcal{L}(\mathcal{H})$ is a compact operator, noted $A \in \mathfrak{S}_\infty(\mathcal{H})$, its eigenvalue sequence is noted $\{\lambda_n\}_{n\in\mathbb{N}}$ counting algebraic multiplicities, and is ordered by non-increasing modulus so that $|\lambda_1(A)| \geq |\lambda_2(A)| \geq \cdots$. Recall that the n-th singular value of $A \in \mathfrak{S}_\infty(\mathcal{H})$ is given by

$$s_n(A) = \sqrt{\lambda_n(A^*A)} = \lambda_n(|A|), \qquad n \in \mathbb{N}, \tag{C.2.1}$$

where $|A| = \sqrt{A^*A}$ and the last inequality follows from the spectral mapping theorem for self-adjoint operators.

We recall that the Schatten-Von Neumman class of operators of order p in $\mathcal{H}$ (in the sequel just p-Schatten), denoted $\mathfrak{S}_p(\mathcal{H})$, consists of all those compact operators in $\mathcal{H}$ whose singular values are p-summable for some fixed $p \in (0, \infty)$. Thus,

$$A \in \mathfrak{S}_p \iff \{s_n(A)\}_{n\in\mathbb{N}} \in \ell^p(\mathbb{N}). \tag{C.2.2}$$

If $1 \leq p < \infty$, it can be shown that $\mathfrak{S}_p(\mathcal{H})$ becomes a Banach space by introducing the p-Schatten norm

$$||A||_p = ||\{s_n(A)\}_{n\in\mathbb{N}}||_{\ell^p}. \tag{C.2.3}$$

Note that in the rhs we are just evaluating the ℓ^p-norm of a sequence, that is, given a sequence $x = \{x_n\}_{n\in\mathbb{N}} \subset \mathbb{C}$, its ℓ^p-norm is $||x||_{\ell^p} = \left(\sum_{n\in\mathbb{N}} |x_n|^p\right)^{1/p}$, and it is the usual Euclidean norm for $p = 2$.

Of particular relevance are the classes $\mathfrak{S}_1$ of trace-class operators and $\mathfrak{S}_2$ of Hilbert-Schmidt operators, see [GGK00, Sim79, Con00] for detailed treatments. If $A \in \mathfrak{S}_1(\mathcal{H})$, its trace is defined as $\mathrm{Tr}A = \sum_n \langle \varphi_n, A\varphi_n\rangle$ for any orthonormal basis $\{\varphi_n\}_n$ of $\mathcal{H}$, and it holds that $\mathrm{Tr}(A) = \sum_n \lambda_n(A)$ (Lidskii's theorem). We will make use of the fact that $\mathfrak{S}_1(\mathcal{H})$ is a two-sided ideal in $\mathcal{L}(\mathcal{H})$, see for instance [Con00] Chapter 3 for proofs.

When we deal with complex matrix spaces of dimension $d \geq 1$, we shall fix the matrix norm to the Frobenius norm[1],

$$||A||_F = \sqrt{\mathrm{Tr}(A^*A)} = \left(\sum_{i,j=1}^{d} |A_{ij}|^2\right)^{1/2}, \qquad A \in \mathbb{C}^{d\times d}. \tag{C.2.4}$$

The generalization of the Frobenius norm is the p-Schatten norm of the matrix, i.e. for $p \geq 1$,

$$||A||_p = \left(\sum_{i=1}^{d} s_i^p(A)\right)^{1/p}. \tag{C.2.5}$$

Note that for $p = 2$ this is just the Frobenius norm.

Recall that two norms $||\cdot||$ and $||\cdot||'$, on a vector space E, are called *equivalent* if there exist numbers $c_1 > 0$ and c_2 such that for all $e \in E$, $c_1||e||' \leq ||e|| \leq c_2||e||'$. Any

[1] Of course here we mean $A^* = A^\dagger$, the conjugate transpose of A.

two norms on a finite dimensional vector space are equivalent (see for instance [GGK03] Chapter XI).

Given a unitary operator $U \in \mathcal{L}(\mathcal{H})$, we denote its associated spectral family by $E_U(\cdot)$, that is

$$\langle \psi, U^n \psi \rangle = \int_{\mathbb{T}} e^{\mathrm{i}n\xi} \mathrm{d}\langle \psi, E_U(\xi)\psi \rangle \tag{C.2.6}$$

for all $\psi \in \mathcal{H}$, $n \in \mathbb{Z}$, $\mathbb{T} = \mathbb{R}/2\pi\mathbb{Z}$. We let $\sigma(U)$ to denote the spectrum of U, $\sigma_p(U)$ the set of its eigenvalues, $\sigma_{sc}(U)$ its singular continuous spectrum, and $\sigma_{ac}(U)$ its absolutely continuous spectrum. If $\sigma(U) = \sigma_{ac}(U)$, then U is said to be purely absolutely continuous, in which case the spectral measure $\mathrm{d}\langle \psi, E_U(\xi)\psi \rangle$ has a Radon-Nikodym derivative with respect to the Lebesgue measure $\frac{\mathrm{d}\langle \psi, E_U(\xi)\psi \rangle}{\mathrm{d}\xi} = F_\psi(\xi)$ that belongs to $L^1(\mathbb{T})$ for any $\psi \in \mathcal{H}$. Recall that the discrete spectrum of U, noted $\sigma_d(U)$, is the set of isolated eigenvalues of finite multiplicity, that is

$$\sigma_d(U) = \{\lambda \in \sigma(U) : \lambda \text{ is an isolated point of } \sigma(T) \text{ and } \dim \text{Ker } (U - \lambda) < \infty\}. \tag{C.2.7}$$

Finally, recall that the essential spectrum is its complement,

$$\sigma_{ess}(U) = \sigma(U) \setminus \sigma_d(U). \tag{C.2.8}$$

The notions (C.2.7) and (C.2.8) are still meaningful for any normal operator, but for general classes of operators the notion of essential spectrum is more subtle, we refer to [Dav07] Chapter 4 for further details.

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